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1995 - 2019

25th ISCB INTERNATIONAL CONFERENCE (ISCBC-2019)

TRENDS IN CHEMICAL AND BIOLOGICAL SCIENCES: IMPACT ON HEALTH AND ENVIRONMENT

12-14 January, 2019

Hotel Golden Tulip, Lucknow, India

ABSTRACT BOOK

Organized by:

Indian Society of Chemists & Biologists (ISCB)

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Vice Chancellor, Gujarat Vidhyapeeth
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Dr. P.M.S. Chauhan
Chief Scientist and Professor,
CDRI, Lucknow
General Secretary, ISCB

Message

We are very happy to inform you that the Indian Society of Chemists and biologists, Lucknow, jointly organising its 25th international conference at Lucknow, India from 12th – 14th January, 2019 (Sat-Mon).

It is a matter of great pleasure that the focal theme of the 25th International Conference of ISCB on "Trends in Chemical and Biological Sciences: Impact on Health and Environment". During above conference researcher are going to discuss self reliance, sustainability & affordability of pharmaceutical substances by improving process chemistry through innovation so that India can be more competitive and self reliant on Pharma products, drug intermediates & finished formulations. Scientists across the globe, especially from USA, Greece UK, France, Poland, Slovenia, Belgium, Sweden, Italy and many other countries will participate as keynote/invited speakers to address above mentioned issues. The entire conference will be addressed by more than 60 senior scientists & professors as key-note/invited speaker while it will attract more than 600 young researchers & post doctoral researchers from entire country who will take part as oral/poster presentations.

We are glad that the scientific committee is bringing out an abstracts book covering the presentations to be made during ISCBC-2019. Our sincere thanks are due to the members of organizing committee. During this conference a number of eminent scientists and technologists of the country and overseas will be discussing the trends, prospects and future directions of research. We look forward to fruitful deliberations in extremely interesting areas of scientific research. We are happy that an extensive and comprehensive scientific program is arranged. The scientific program beside inaugural function includes 1 Keynote lecture, 14 plenary lectures, 44 invited lectures by the eminent scientists from India and abroad. 32 Oral presentations by the young researchers are scheduled. The most heartening feature of the conference is that it is being participated with a number of young scientists and Ph. D. students and presentations are schedules in three poster sessions. On behalf of ISCB we are looking for the galaxy of speakers and young participants who made this conference a memorable event. We extend our warm welcome to all National and International delegates from pharmaceutical companies, research organization, universities and academic institutes wish them very happy stay at Jaipur. Now Finally I take this opportunity to express my sincere thanks and gratitude to members and office bearers of organizing committee of 25th International Conference (ISCBC-2019).

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SCIENTIFIC PROGRAMME

Saturday, January 12, 2019

9.00 AM - 10.30 AM	**Registration**
10.30 AM - 12.00 PM	**Inaugural Session**
12.00 PM - 12.30 PM	**High Tea**

Session – I
Chairpersons: Prof. Anamik Shah and Dr. Mukund S. Chorghade

PL-1 12.30 PM - 1.00 PM	**Colin J Suckling** Research Professor of Chemistry, Department of Pure & Applied Chemistry, University of Strathclyde, Glasgow, Scotland **Minor Groove Binders (S-MGBs) - Pluripotent Anti-infective compounds to tackle antimicrobial resistance**
PL-2 1.00 PM - 1.30 PM	**Athina Geronikaki** Department of Pharmaceutical Chemistry, Aristotle University, Greece **Docking assisted design of novel 4-adamantanyl-2-thiazolylimino-5-arylidene-4-thiazolidinones as potent NSAIDs**
1.30 PM - 2.30 PM	**Lunch**

Session – II
Chairpersons: Dr. Keshav Deo and Dr. Babita Malik

PL-3 2.30 PM - 2.55 PM	**Tapas K. Kundu** Director, CSIR-Central Drug Research Institute, Lucknow, India **Chemical Biology Approach to Understand Differentiation and Disease: Implication in Therapeutics**
IL-1 2.55 PM - 3.15 PM	**Mukund S. Chorghade** President and Chief Scientific Officer, THINQ Pharma / THINQ Discovery, and Chorghade Enterprises, USA **Fascinating Adventures in Development of a Drug from Conception to Commercialization: A Personal Perspective**
IL-2 3.15 PM - 3.35 PM	**Arun K. Sinha** Chief Scientist and Professor (AcSIR), Medicinal and Process Chemistry Division, CSIR-Central Drug Research Institute, Lucknow, India **Abstract Awaited**
IL-3 3.35 PM - 3.55 PM	**Ashok K Prasad** Professor, Department of Chemistry, University of Delhi, Delhi, India **Abstract Awaited**
IL-4 3.55 PM - 4.15 PM	**Hitendra. M. Patel** Department of Chemistry, Sardar Patel University, Vallabh Vidyanagar, Gujarat, India

	An efficient one-pot multicomponent synthesis of Diverse Heterocyclic Scaffolds and their Biological importance
IL-5 4.15 PM - 4.35 PM	**Ashoke Sharon** Department of Chemistry, Birla Institute of Technology, Mesra, Ranchi, India **Carbocyclic derived analogs: A promising scaffold towards discovery of antiviral drug like nucleoside**
4.35 PM - 4.50 PM	**Tea**

Session – III
Chairpersons: Prof. N.C. Desai and Prof. Devendra Kumar

PL-4 4.50 PM - 5.15 PM	**Ram A Vishwakarma** Director, CSIR-Indian Institute of Integrative Medicine, Jammu, India **Abstract Awaited**
IL-6 5.15 PM - 5.35 PM	**Dalip Kumar** Department of Chemistry, Birla Institute of Technology and Science, Pilani, India **Efficient Syntheses of Drug-like Nitrogen Heterocycless**
IL-7 5.35 PM - 5.55 PM	**Naresh Chandra Bal** Ramalingaswami Fellow, School of Biotechnology, KIIT University, Bhubaneswar, India **Searching a target to treat metabolic syndrome: Brown fat or the muscle?**
IL-8 5.55 PM - 6.15 PM	**Manik Pradhan** S N Bose National Centre for Basic Sciences, Kolkata, India **New frontiers in gas-phase cavity ring-down spectroscopy for medical diagnosis and environmental sensing**
IL-9 6.15 PM - 6.35 PM	**Brijesh Kumar** Senior Principal Scientist, Sophisticated Analytical Instrument Facility (SAIF), CSIR- Central Drug Research Institute, Lucknow, India **Applications of LC- MS tools in natural products**

5.35 PM – 7.00 PM	**Poster Session -I (Poster Numbers 1-60)**
7.00 PM – 8.30 PM	**Cultural Programme**
8.30 PM	**Dinner**

Sunday, January 13, 2019

Parallel Session – IVA (Ivy Hall, Ground Floor)
Chairpersons: Dr. Rakesh Shukla and Prof. S. K. Singh

PL-5 9.00 AM - 9.30 AM	**Jyoti Chattopadhyaya** Department of Cell & Molecular Biology, Biomedical Center, Uppsala University, Uppsala, Sweden **Specific Destruction of Virus and Oncogenein Human cellby Designed Small Interfering RNA**

PL-6 9.30 AM - 10.00 AM	**S. J. S. Flora** Director, National Institute of Pharmaceutical Education and Research (NIPER), Raebareli, India **Abstract Awaited**
IL-10 10.00 AM - 10.20 AM	**Parthasarathi Das** Associate Professor, Department of Applied Chemistry, Indian Institute of Technology (ISM), Dhanbad, India **Abstract Awaited**
IL -11 10.20 AM - 10.40 AM	**Dipankar Koley** Scientist, CSIR-Central Drug Research institute, Lucknow, India **Privileged Scaffold Diversification through C–H bond functionalization using 1st Row Transition Metals-catalysts**
IL -12 10.40 AM - 11.00 AM	**Bapu B. Shingate** Assistant Professor, Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University, Aurangabad, India **Tips for Effective Preparation of Scientific Reviews**
IL -13 11.00 AM -11.20 AM	**Indresh Kumar** Department of Chemistry, Birla Institute of Technology and Science, Pilani, Pilani-campus (Rajasthan), India **Linear dicarbonyls as suitable substrates for amine catalyzed transformations: Synthesis of medium-sized N-heterocyclic compounds**
11.20 AM - 11.40 PM	**High Tea**

Parallel Session – IVB (Daffodil Hall, Sixth Floor)
Chairpersons: Prof. R. K. Singh and Dr. Arunava Agarwala

IL-14 9.00 AM - 9.15 AM	**Anand S. Aswar** Department of Chemistry, Sant Gadge Baba Amravati University, Amravati, India **A simple synthesis of transition metal nanocrystalline ferrite:An effective and environmentally benign catalystfor the one-pot multicomponentreactions**
IL-15 9.15 AM - 9.30 AM	**Amit Kumar** Indian Institute of Technology Patna, Bihta, Patna- Bihar, India **Imidates: A Versatile Synthons for Organic Chemists**
IL-16 9.30 AM - 9.45 AM	**Neelima Gupta** Associate Professor, Department of Chemistry, University of Rajasthan, Jaipur, India **Dienophilicity of >C=P– Functionality of 2-Phosphaindolizines towards Electron Rich Vs Electron Deficient Dienes**
IL -17 9.45 AM - 10.00 AM	**Surendra Singh** Assistant Professor, Dept. of Chemistry, University of Delhi, Delhi, India **Development of Chiral Catalysts for Asymmetric Aldol and Henry Reactions**
IL -18 10.00 AM - 10.15 AM	**Venkata Ramana Doddi** Assistant Professor, Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University, Aurangabad, India

	The triple role of 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU) in the synthesis of diaryl ethynes and enynes from 1,1-dibromoalkenes at ambient temperature
IL -19 10.15 AM -10.30 AM	**Vikas Tyagi** School of Chemistry and Biochemistry, Thapar Institute of Engineering and Technology, Patiala, Punjab, India **Myoglobin-catalyzed olefin-cyclopropanation reaction**
O -1 10.30 AM -10.40 AM	**Sarvesh Kumar Pandey** Department of Chemistry, Indian Institute of Technology, Kanpur, India **Quantification of Hydrogen Bond Strength Based on Interaction Coordinates: A New Approach**
O -2 10.40 AM -10.50 AM	**Shikha Awasthi** Department of Material Science and Engineering, Indian Institute of Technology, Kanpur, India **Synergistic Role of Carbonaceous Reinforcements on Multi-Length Scale Tribology of Electrophoretically Deposited Nickel-Boron Nitride Coatings**
O -3 10.50 AM -11.00 AM	**Siddharth Bhoraskar** Department of Chemistry, University of Massachusetts at Lowell, Massachusetts, USA **Biochemical Characterization ofFc-Fusion Protein Conformers**
O -4 11.00 AM -11.10 AM	**Shabi Abbas Zaidi** Department of Chemistry, Kwangwoon University, 20 Kwangwoon-ro, Nowon-gu, Seoul, South Korea **Electrospun woven antibacterial wound healing mats synthesized with norfloxacin imprinted polymer nanofibers**
O -5 11.10 AM -11.20 AM	**Himanshu Arora** India **Copper (II) dimers stabilized by bis(phenol) amine ligands: Theoretical and Experimental Insights**
11.20 AM - 11.40 PM	**High Tea**

Parallel Session-VA (Ivy Hall, Ground Floor)
Chairpersons: Dr. S.K. Puri and Dr. PMS Chauhan

PL-7 11.40 AM - 12.05 PM	**Kazuaki Matsumura** Associate Professor, School of Materials Science, Japan Advanced Institute of Science and Technology, 1-1 Asahidai, Nomi, Ishikawa, Japan **BIOMEDICAL MATERIALS APPLICATION OF POLYAMPHOLYTES**
PL-8 12.05 AM - 12.30 PM	**Madhu Dikshit** Former Director, CSIR-Central Drug Research Institute, Lucknow, India **Abstract Awaited**
PL-9 12.30 AM - 12.55 PM	**Rakeshwar Bandichhor** Director and CoE-Chemistry Head-API-R&D,Vice Chair, ACS-India Chapter (South), Dr. Reddy's Laboratories,Hyderabad, India **Innovative Process Research and Development of APIs**

IL-20 12.55 PM - 1.15 PM	**Ramesh Babu Boga** BogaR Laboratories LLC, Suwanee, GA, USA **Newer Trends of Drug Discovery: Current Status of Nitric Oxide Synthase (NOS) Inhibitors**
IL-21 1.15 PM - 1.30 PM	**Debasish Mandal** School of Chemistry and Biochemistry, Thapar Institute of Engineering and Technology, Patiala, Punjab, India **Myoglobin Reconstitutedwith Manganese Porphycene – A Promising Bio-catalyst for C-H Activation: An insight into the Theoretical Investigation**
IL-22 1.30 PM - 1.45 PM	**Sharad Porwal** Chemical Sciences Research Group, Division of Research and Development, Lovely Professional University, Phagwara, Punjab, India **Coupling slow H_2S donors with drug fragments: A new strategy in discovering low toxicity drugs**
1.45 PM - 2.30 PM	**Lunch**

Parallel Session-VB (Daffodil Hall, Sixth Floor)
Chairpersons: Dr. R.P. Tripathi and Dr. Anshu Dandia

IL-23 11.40 PM - 12.00 PM	**Diwan S Rawat** Coordinator, M. Tech (Chemical Synthesis and Process Technologies), Department of Chemistry, University of Delhi, Delhi, India **Identification of lead antimalarial and anti-Parkinson molecule *viamolecular* hybridization approach**
O-6 12.00 PM - 12.10 PM	**Amit Rajput** Department of Basic and Applied Science, G. D. Goenka University, Gurgaon, Haryana, India **Six-coordinate $[Co^{III}(L)2]^z$ complexes (L(2–) = azo-ppended *o*-aminophenolate; z = 1–, 0, 1+): molecular and electronic structure**
O-7 12.10 PM - 12.20 PM	**Neelam Yadav** Department of Medicine, Albert Einstein College of Medicine, Bronx, New York, USA **Survival and proliferation improves of liver sinusoidal endothelial cells transplanted in mice by endothelin receptor antagonism**
O-8 12.20 PM - 12.30 PM	**Pratibha Yadav** Centre for Rural development and Technology, IIT Delhi, Hauz Khas, New Delhi, India **Ascorbate peroxidase and its role in the transformation of methyl phenyl sulfide to its sulfoxide**
O-9 12.30 PM - 12.40 PM	**Bharat Chandra Sahu** Department of Chemistry, VEC Lakhanpur, Sarguja University, Ambikapur, C.G, India **Baylis–Hillman Acetates in Synthesis: Copper(I)/tert-Butyl Hydroperoxide Promoted One-Pot Oxidative Intramolecular Cyclization Protocol for the Preparation of Pyrrole-Fused Compounds and the Formal Synthesis of (±)-**

O-10 12.40 PM - 12.50 PM	**Mayank G. Sharma** Department of Chemistry, Sardar Patel University, Vallabh Vidyanagar, Gujarat, India **Green approach for the synthesis of 1, 4-dihydropyridine moiety and their biological assay**
O-11 12.50 PM - 1.00 PM	**Neha Gupta** Department of Chemistry, UGC Sponsored-Centre for Advanced Studies-II, Guru Nanak Dev University, Amritsar, Punjab, India **Designing of Smart Fluorescent Probes for Bio-imaging and Diagnostics**
O-12 1.00 PM - 1.10 PM	**ChandralataBal** Department of Chemistry, Birla Institute of Technology, Mesra, Ranchi, India **Rhodium catalyzed stereospecific reductivecarbocyclization of 1,6-enynes for the synthesis of entecavir-aristromycin hybrid analogs**
O-13 1.10 PM - 1.20 PM	**Nivedita Jena** KIIT Technology Business Incubator, KIIT University, Bhubaneswar, Odisha, India **Startup Opportunities in Chemistry-Biology Interface**
O-14 1.20 PM - 1.30 PM	**Dodla Sivanageswara Rao** Department of Chemistry, Malaviya National Institute of Technology(MNIT), Jaipur, Rajasthan, India **Chemoselective Iodination of Alkynes using Sulfonium Iodate (I) Complex**
O-15 1.30 PM - 1.40 PM	**ThurpuRaghavendar Reddy** Department of Chemistry, Malaviya National Institute of Technology, (MNIT), Jaipur, Rajasthan, India **Sulfonium Iodate Reagent MediatedStereoselectiveSynthesis of 2-Deoxy Glycosidesand Glycoconjugates**
O-16 1.40 PM - 1.50 PM	**Abhay J Bavishi** Christ College, Rajkot, Vidyaniketan, Rajkot, India **Novel, facile and green approach towards synthesis of Imidazolocoumarin derivative**
1.50 PM - 2.30 PM	**Lunch**

Parallel Session – VIA (Ivy Hall, Ground Floor)
Chairpersons: Prof. Jyoti Chattopadhyay and Prof. Raja Roy

PL-10 2.20 PM - 2.45 PM	**Anil Kumar Singh** IIT Mumbai, Former Vice Chancellor, University of Allahabad, India **Understanding Rhodopsins through Bioorganic Chemistry**
IL-24 2.45 PM - 3.05 PM	**Bakrudeen Ali Ahmed** Faculty of Applied Sciences, Ton Duc Thang University, Ho Chi Minh City, Vietnam **Plant Biotechnology Products:Bio-safety and health security**
IL-25 3.05 PM - 3.25 PM	**Dhananjay V Mane** Professor in chemistry and Regional Director, Yashvantrao Chavan Maharastra Open University, Nashik, India

	ANTI-INFLAMMATORY EXPLORATION OF SULFONAMIDE CONTAINING DIARYL PYRAZOLES WITH PROMISING COX-2 SELECTIVITY AND ENHANCED GASTRIC SAFETY PROFILE
IL-26 3.25 PM - 3.45 PM	**T. Narender** Principal Scientist, Medicinal and Process Chemistry Division, CSIR-Central Drug Research Institute, Lucknow, India **Aegeline inspired synthesis of novel β3-AR agonists for insulin resistance and Amino alcohol and thiazolidinedione hybrids for antiadipogenic activity**
IL-27 3.45 PM - 4.00 PM	**Sushil K. Maurya** Natural Product Chemistry and Process Development Division, CSIR-Institute of Himalayan Bioresource Technology, Palampur, Himachal Pradesh, India **Method development for C-N bond formation and their applications in medicinal chemistry**
O-17 4.00 PM - 4.10 PM	**Debasis Manna** Department of Chemistry, Indian Institute of Technology Guwahati, Guwahati, Assam, India **Diphenylethylenediamine-Based Potent Anionophores: Transmembrane Chloride Ion Transport and Apoptosis Inducing Activities**
O-18 4.10 PM - 4.20 PM	**Rahul Shivahare** Division of Parasitology, CSIR-Central Drug Research Institute, Lucknow, India **Synergism between Novel Immunomodulators and Chemotherapy for the Cure of Experimental Visceral Leishmaniasis**
O-19 4.20 PM - 4.30 PM	**Ramprasad O.G.** Aravind Medical Research Foundation, Madurai, India **EXPLORATION OF A NOVEL CHEMICAL CROSS-LINKER FOR THE TREATMENT OF KERATOCONUS**
4.30 PM - 4.40 PM	**Tea**

Parallel Session – VIB (Daffodil Hall, Sixth Floor)
Chairpersons: Prof. Mahesh Sharma and Prof. Manjunath Ghate

IL-28 2.20 PM - 2.40 PM	**Virinder S Parmar** Bioorganic Laboratory, Department of Chemistry, University of Delhi, Delhi, India **Novel Polymeric Antioxidants and Bio-Antioxidants: Our Extensive Studies**
IL-29 2.40 PM -3.00 PM	**Anil Kumar** Department of Chemistry, Birla Institute of Technology and Science, Pilani, India **Transition-Metal-Free Approaches for the Synthesis of Heterocycles and Functionalization of sp^3/sp^2 C–H Bonds**
O-20 3.00 PM - 3.10 PM	**Ranjan C Khunt** Department of Chemistry, Saurashtra University, Rajkot, (Gujarat) India **Synthesis of 1, 5-disubstituted Tetrazole Derivatives via a TMS-N_3 Based Ugi Reaction as Anti-cancer Agents and their Docking Study**
O-21 3.10 PM - 3.20 PM	**Roli Mishra** Chemistry Department, Centre for Engineering and Enterprise Institute of Advanced Research, Gandhinagar, India

	Amino acid- Imidazolium Ionic Liquids: Synthesis and Application
O-22 3.20 PM - 3.30 PM	**Om P. S. Patel** Department of Chemistry, Birla Institute of Technology and Science Pilani, Pilani Campus, Rajasthan, India ***tert*-Butyl Hydroperoxide as Carbon Source and Hydrogen Ac-ceptor: Regioselective Aminomethylation of Imidazoheterocycles with 2/4-Aminoazaheterocycles *via* Cross-Dehydrogenative Coupling**
O-23 3.30 PM - 3.40 PM	**Ramhari Meena** Department of Chemistry, University of Rajasthan, JLN Marg, Jaipur, Rajasthan, India **Synthesis, characterization and anticancer activity of Pt(II) and Pd(II) complexes with Schiff base ligands**
O-24 3.40 PM - 3.50 PM	**Abu Salim Mustafa** Departments of Microbiology and Medicine, Faculty of Medicine, Health Sciences Centre, Kuwait University, Kuwait **DISTRIBUTION OF VITAMIN D BINDING PROTEIN SUBTYPES IN KUWAITI POPULATION**
O-25 3.50 PM - 4.00 PM	**Rajesh Kumar** Department of Chemistry, R.D.S. College (B.R.A. Bihar University), Muzaffarpur, India **Chemo-enzymatic Synthesis of Modified Nucleosides**
O-26 4.00 PM - 4.10 PM	**Sundaram Singh** Department of Chemistry, Indian Institute of Technology, Banaras Hindu University, Varanasi, India **An Efficient and Sustainable Synthesis of Substituted spirooxindoles via Monoclinic nanozirconia catalyzedMulticomponent reaction of Isatin derivatives with Ethylcyanoacetate and 1,3-dicarbonyl compounds in a Ball mill**
O-27 4.10 PM - 4.20 PM	**Dinesh Kumar** Centre of Biomedical Research (CBMR), SGPGIMS Campus, Lucknow, India **Quercetin, a Natural Flavonoid with Anti-Helicobacter pylori Activity, interacts with its Histone-like DNA binding protein: A promising candidate for developing next generation anti-H. pylori agents**
O-28 4.20 PM - 4.30 PM	**Susruta Samanta** Manipal University Jaipur, Dehmi-Kalan, Jaipur-Ajmer Expressway, RJ, India **Translocation of antibiotics through the outer membrane channel OprE of *Pseudomonas aeruginosa***
4.30 PM - 4.40 PM	**Tea**

Parallel Session – VIIA (Ivy Hall, Ground Floor)
Chairpersons: Prof. N.C. Desai and Dr. A.K. Dwivedi

PL-11 4.40 PM - 5.05 PM	**Anna Kajetanowicz** Biological and Chemical Research Centre, Faculty of Chemistry, University of Warsaw, Poland **Macrocyclisation at high concentration and other problems in olefin metathesis:**

	looking for solutions
IL-30 5.05 PM - 5.25 PM	**Namrata Rastogi** Medicinal & Process Chemistry Division, CSIR-Central Drug Research Institute, Lucknow, India **Evolution & Interweaving of Diazo Group Chemistry with Visible Light Catalysis**
IL-31 5.25 PM - 5.45 PM	**Ram Sagar Misra** Associate Professor, Department of Chemistry, Banaras Hindu University, Varanasi, India **Stereoselective Synthesis of Natural Product Inspired Carbohydridsas Antiproliferative Agents**
IL-32 5.45 PM - 6.00 PM	**Luxami, V.** School of Chemistry and Biochemistry, Thapar Institute of Engineering and Technology, Patiala, India **ESIPT based Hydroxy-aryl benzimidazoles/Schiff bases as chromo fluorescent sensor and logic devices**
IL-33 6.00 PM - 6.20 PM	**B. K. Singh** Department of Chemistry, University of Delhi, North Campus, Delhi, India **Metal-Free Approaches for the Construction of C-C and C-N Bonds**
IL-34 6.20 PM - 6.40 PM	**Dina Nath Singh** Associate Professor, K.S. Saket PG College, Dr. Ram Manohar Lohia Avadh University, Faizabad, India **Current status leading to the discovery of drugs from medicinal plants**
O-29 6.40 PM - 6.50 PM	**Ranjay Shaw** Department of Chemistry, University of Delhi, North Campus, Delhi, India **Transition metal free chemoselectivesynthesis of isolated and fused fluorenone and study of their photophysical properties**
O-30 6.50 PM - 7.00 PM	**Hossain, M. S.** University of South Bohemia in České Budejovice, Faculty of Fisheries and Protection of Waters, Zátiší 728/II, Vodňany, Czech Republic **Environmentally relevant concentrations of psychotropic drugsmodify the behavioural patterns of an aquatic invertebrate**

Parallel Session – VIIB (Daffodil Hall, Sixth Floor)
Chairpersons: Dr. Nighat Fahmi and Dr. Ashok K. Prasad

PL-12 4.40 PM - 5.05 PM	**Alok Dhawan** Director, CSIR-Indian Institute of Toxicology Research, Lucknow, India **Abstract Awaited**
IL-35 5.05 PM - 5.25 PM	**Ellis O'Neill** Department of Plant Sciences, University of Oxford, Oxford, UK **Antibiotics from pond scum – exploring natural product biosynthesis in algae**
IL-36 5.25 PM - 5.45 PM	**Rajeev Sakhuja** Department of Chemistry, Birla Institute of Technology and Science, Pilani,

	Rajasthan, India **Harvesting fused & functionalized azaheterocycles *via* metal-catalyzed and metal-free strategies: Promising pharmacophores for drug development**
IL-37 5.45 PM - 6.05 PM	**Hemant Joshi** Department of Chemistry, Birla Institute of Technology and Science, Pilani, Rajasthan, India **Dibridgehead Diphosphine Cage as Molecular Receptor for Precious Metal Capture and Transport**
IL-38 6.05 PM - 6.25 PM	**Ramendra Pratap Singh** Department of Chemistry, University of Delhi, North Campus, Delhi, India **Synthesis of various arylated benzenes from 2-(1-arylethylidene)-malononitriles**
O-31 6.25 PM - 6.35 PM	**Amr Elagamy** Department of Chemistry, University of Delhi, North Campus, Delhi, India **Synthesis of Highly Functionalized Spirobutenolidesvia Nitroalkane Mediated Ring Contraction of 2-Oxobenzo[*h*]chromenes through Denitration**
O-32 6.35 PM - 6.45 PM	**Komal M. Vyas** Department of Chemistry, Sardar Patel University, Vallabh Vidyanagar, Gujarat, India **Synthesis, characterization and biological significance of Cu(II) complexes bearing heterocyclic ligands**
O-32 6.45 PM - 6.55 PM	**Rohit Singh** Medicinal and Process Chemistry Division, CSIR-Central Drug Research Institute, Lucknow, India **In *vitro* Anti-hyperglycaemic activity of 4-hydroxyisoleucine derivatives**

7.00 PM – 8.00 PM	**Poster Session -II (Poster Numbers 61 onwards)**
8.00 PM	**Dinner**

Monday, January 14, 2019

Session –VIII
Chairpersons: Prof. Ganesh Pandey and Dr. Rahul Shrivastava

PL-13 9.00 AM – 9.25 AM	**Surya Kant** Professor & Head, Dept. of Respiratory Medicine and Pulmonary & Critical Care Medicine (Off.), King George's Medical University, Lucknow, India **TB Free India by 2025: Roadmap to Prime minister's Dream**
PL-14 9.25 AM -9.50 AM	**C.L. Khetrapal** Centre of Biomedical Magnetic Resonance, Sanjay Gandhi PGI Campus, Lucknow, India **NMR in Chemistry, Biology, Health Sciences and beyond**
IL-39 9.50 AM - 10.10 AM	**N. C. Desai** Division of Medicinal Chemistry, Department of Chemistry, Mahatma Gandhi Campus, Maharaja Krishnakumarsinhji Bhavnagar University, Bhavnagar, India

	Fluorine Chemistry–An important tool for new drug discovery program in the 21st century
IL-40 10.10 AM - 10.30 AM	**Makarand Waikar** ACS International India Pvt. Ltd., Pune, India **Science and Technology trends in Biologics**
IL-41 10.30 AM - 10.50 AM	**Om Prakash** Professor and Director, Mary L. Vanier Biomolecular NMR Facility, Dept. of Biochemistry and Molecular Biophysics, Kansas State University, Manhattan, USA **Bacteria Fighting Back: Structural Basis for Function of the Staphylococcal Peroxidase Inhibitor**
IL-42 10.50 AM -11.10 AM	**Satpal Singh Badsara** Assistant Professor, Centre of Advanced Study, Department of Chemistry, University of Rajasthan, Jaipur, India **Open flask, catalyst-free synthesis ofoxindole containing α-hydroxy phosphinoyl compounds**
IL-43 11.10 AM -11.30 AM	**Ravindra Kumar** Medicinal and Process Chemistry, CSIR-Central Drug Research Institute (CDRI), Lucknow, India **Enantioselective Unified Oxidative Cyclization strategy to Diverse Carbocyclic scaffolds**
IL-44 11.30 PM -11.50 PM	**Devdutt Chaturvedi** Department of Chemistry,School of Physical & Material Sciences, Mahatma Gandhi Central University (MGCU), Distt.: East Champaran, Bihar, India **Versatility of carbon disulfide: Greener synthetic strategies for biologically potent scaffolds**
11.50 AM - 12.10 PM	**High Tea**

12.10 PM - 1.30 PM	**Valedictory Session**

1.30 PM – 2.30 PM	**Lunch**

- End of Programme -

PLENARY

PL-1

Strathclyde Minor Groove Binders (S-MGBs) - Pluripotent Anti-infective compounds to tackle antimicrobial resistance.

Professor Colin Suckling

WestCHEMDepartment of Pure and Applied ChemistryUniversity of Strathclyde Glasgow Scotland

The threat of antimicrobial resistance to existing drugs exists across the breadth of infective agents including bacteria, fungi, and parasites which together are responsible for debilitating and fatal diseases to human and animal populations world-wide. The conventional medicinal chemistry response to this challenge is to identify specific target proteins in the infectious agent for new drugs binding to which would lead to selective toxicity, an approach that is continuously under investigation in industrial and academic laboratories. This strategy, however, runs the immediate risk that on introduction of the new medicine the infectious agents will adapt leading to the rapid emergence of resistant strains, as has happened widely before. A strategy more resilient to the emergence of resistant strains might have major advantages for the discovery of new drugs in today's AMR era. Such a strategy would require multitargeting of a new drug molecule and the most economical way of achieving this is to target DNA. A drug binding to DNA can in principle switch off many biological pathways so that the probability of resistance emerging rapidly is greatly reduced. Provided ways can be found to avoid toxicity to the patient, animal or human, such compounds are attractive as potential anti-infectives.

The Minor Groove Binders project at the University of Strathclyde was begun with the above strategy in mind and has led to the synthesis of over 400 compounds (S-MGBs). Subsets of compounds with high activity against some bacteria (Gram positive, mycobacteria), fungi (Candida spp. and Aspergillus spp.), and parasites (Plasmodia spp., Trypanosoma spp. and Leishmania spp.) have been identified and the structures are being optimized for the various applications. One antibacterial compound for the treatment of *Clostridum difficile* infections has reached a Phase 2 clinical trial. Potential clinical candidates for the treatment of fungal infections and animal trypanosomiasis have also been identified. This presentation will explore aspects of the activity of S-MGBs in various applications including mechanism of action studies, resilience to the development of resistance, and selectivity.

PL-2

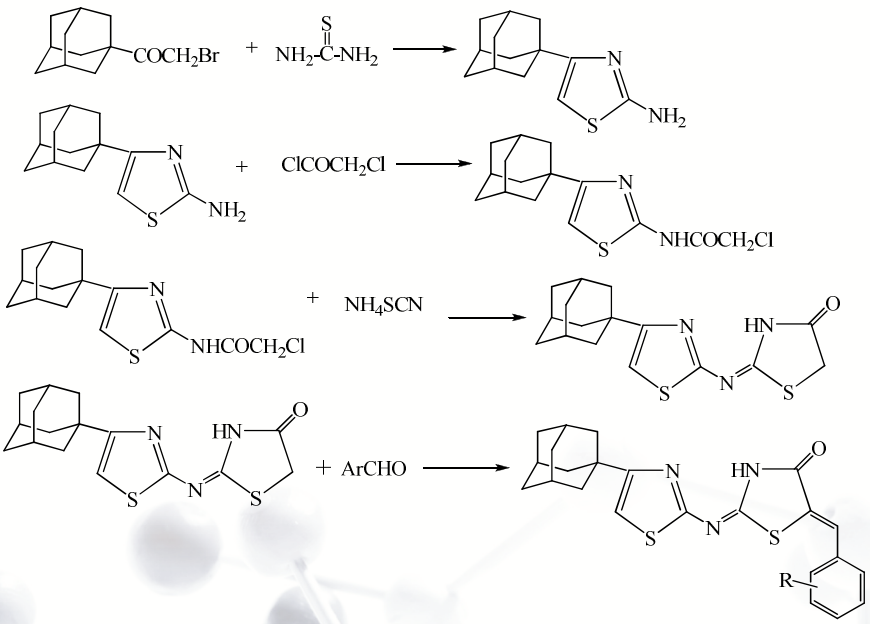
Docking assisted design of novel 4-adamantanyl-2-thiazolylimino-5-arylidene-4-thiazolidinones as potent NSAIDs

Kouatly O[1]., Eleftheriou Ph[2]., Petrou A[1]., Hadjipavlou-Litina D[1]., Geronikaki A[1]*.

[1]*Department of Pharmaceutical Chemistry , School of Pharmacy, Aristotle University of Thessaloniki, 54124, Greece.*
[2]*Department of Medical Laboratories, School of Health and Care Professions, Alexandrion Technological Educational Institute of Thessaloniki, Greece.*

Docking analysis was used to predict the effectiveness of adamantanyl insertion in improving COX/LOX inhibitory action of previously tested 2-thiazolylimino-5-arylidene-4-thiazolidinones. The crystal structure data of human 5-LOX (3O8Y) and ovine COX-1 (1EQH) and mouse COX-2 (3ln1) were used for docking analysis. All docking calculations were carried out using software AutoDock 4.2.

Following prediction results, eleven adamantanyl derivatives were synthesized as presented in Scheme 1and evaluated for biological action. Prediction results correlated well with biological evaluation. Comparison of the novel adamantanyl derivatives with the 2-thiazolylimino-5-arylidene-4-thiazolidinones previously tested showed that insertion of adamantanyl group led to the production of more potent COX-1 inhibitors, as well as LOX inhibitors (increased activity from 200% to 560%). Five compounds out of the eleven exhibited better activity than naproxen; nine out of eleven showed better activity than NDGA, and seven compounds possessed better anti-inflammatory activity than indomethacin.



Scheme 1. Synthesis of title compounds.

PL-3

Chemical Biology Approach to Understand Differentiation and Disease: Implication in Therapeutics

Tapas K. Kundu

Director, CSIR-Central Drug Research Institute, Lucknow, India

PL-4

Ram A Vishwakarma

Director, CSIR-Indian Institute of Integrative Medicine, Jammu, India

Abstract Awaited

PL-5

Specific Destruction of Virus and Oncogenein Human cell by Designed Small Interfering RNA

Jyoti Chattopadhyaya

Department of Cell & Molecular Biology, Box 596, Biomedical Center, Uppsala University, 75124 Uppsala, Sweden
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Our carba-LNA modified antisense and siRNA oligos have been shown to accomplish knockdown of disease-specific oncogene mRNA with (1) high blood-serum stability>500 times, (2) enhanced mRNA affinity, and (3) higher than native RNase and RISC recruitment and cleavage rate, as shown by (i) successful 70-80% knockdown of the papilloma virus (HPV18) oncogenic E6 mRNA at its splice site, at 1.3nM of siRNA, resulting an enhanced p53 protein and apoptosis level, (ii) inhibition of mutant Huntington protein (HTT) against expanded CAG repeat (IC50 = 15 nM) with 7-fold more selectivity, as well as (iii) by inhibition of translation of TAR1 RNA of HIV (IC50 = 0.1 nM). Biggest caveats for successful oligo-therapeutics are: poor cell delivery/cellular-uptake, cellular-stability and off-target effects, which are addressed by new carba-LNA modified oligo-conjugates with specific delivery functions and fluorescent-tracking ligands to monitor oligo-transport and internalization. For this, we are making siRNA-conjugates with cell-type specific peptides and/or small active molecules, which bind to defined immune cell-specific receptor(s) with high affinity, in order to promote faster cleavage/turnover of target mRNA in DICER and RISC. Non-cleavable siRNAs will be used to study Dicer and Ago2 protein by NMR and X-ray to reveal structure-function relations in the ternary complex, which we aim to exploit in the design of smart siRNAs to engineer more effective target mRNA degradation in RISC.

Reference:

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3. Chattopadhyaya*et al. Chem. Rev.***2012**,*112*, 3808; *J. Org. Chem.* **2011**,*76*,4408; *J. Org. Chem.***2012**,*77*, 6855; *J. Org. Chem.***2009**,*74*, 3248; *J. Am. Chem. Soc*.**2007**,*129*, 8362; *Curr. Opin. Drug Disc. Dev*. **2009**, *12*, 876) to aid **cell delivery, stability and RNA targeting i*n vitro* / *in vivo* models**includinginfection model of infection-associated cancers (*Cell*, **2008** *134*, 577,Science 319(5866), 1096–1100

PL-6

S. J.S. Flora

Director, National Institute of Pharmaceutical Education and Research (NIPER), Raebareli, India

Abstract Awaited

PL-7

BIOMEDICAL MATERIALS APPLICATION OF POLYAMPHOLYTES

Kazuaki Matsumura

Japan Advanced Institute of Science and Technology

Polyampholytes are polymers that carry both positive and negative charges. There are two types of polyampholytes: one in which the existence of positive and negative charges is owing to the presence of anionic and cationic monomers, and one in which the presence of a zwitterion is responsible for both charges. The term polyampholytes refers to a broad array of polymers including both types mentioned above; however, in recent times, zwitterionic polymers in themselves have emerged as a new class of polymers. The main difference between the two types of polyampholytes is that in the former case, the charge of the polymer backbone can be easily changed or tuned by changing the ratio of the two monomers. Thus, in these polymers, one charge can dominate and the net charge of the polymer may be either positive, negative or zero. However, in zwitterionic polyampholytes, the net charge is usually zero under normal conditions because of the presence of an equal number of positive and negative charges. This type of polyampholyte displays a hybrid-like property profile owing to the presence of a high population of polymer-bound ion pairs attached to the polymer chain.

Recently, we showed that polyampholytes can be effective cryoprotective agents (CPAs). They introduced a negative charge in a cationic bio-based polymer, ε-poly-L-lysine (ε-PLL), by using succinic anhydride (SA). ε-PLL is an L-lysine homopolymer biosynthesized by Streptomyces species. It is used as a food additive owing to its antimicrobial activities ascribed to the cationic charge density of its side-chain α-amino groups. At an appropriate cation to anion charge ratio (65% of the α-amino groups were converted into carboxyl groups), the polyampholytes showed remarkable CPA efficacy and cells exhibited a viability after freezing that was significantly higher than that with dimethyl sulfoxide (DMSO).

We reported that the zwitterionic polymer poly-sulfobetaine (poly-SPB) showed very high activity in inhibiting the thermal aggregation of lysozyme. This was the first report of a zwitterionic polymer being used to suppress in vitro protein aggregation.

In the application of self-assembled polyampholyte nanoparticles for materials delivery, various factors such as size, surface properties, specificity towards cells, and most importantly, endosomal escape property could play a pivotal role in successful outcome of drug therapy. In addition, self-assembled polyampholyte nanocarriers show good biocompatibility, excellent stability, and high drug adsorbance. These carriers are easy to modify, have high responsiveness and ability to deliver drugs to their target site across biological barriers, and can prolong the circulation time of the encapsulated drugs. The development of polyampholyte-based biomaterials will continue to attract much interest and the NPs possess good potential in various biomedical treatments and basic technologies in future.

Keywords: [biomaterials, polymer, bioactive polymers]

PL-8

Madhu Dikshit

Former Director, CSIR-Central Drug Research Institute, Lucknow, India

Abstract Awaited

PL-9

Innovative Process Research and Development of APIs

Rakeshwar Bandichhor

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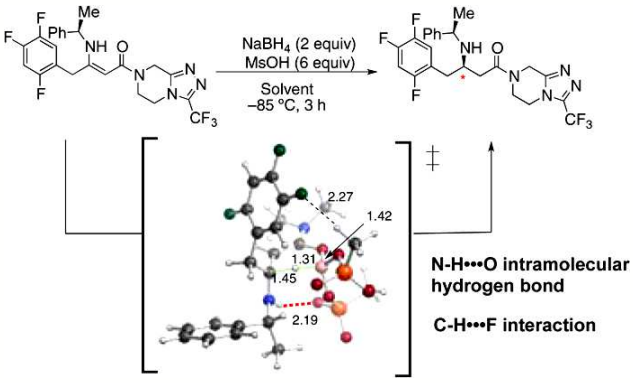
Abstract : As a healthcare requirement to have affordable medicines led to an explosive growth of the branded/generic pharmaceutical industries in recent past. Quite evidently, the pharmaceutical production has come with a significant irreparable environmental damage. As a result, pharmaceutical industry turns out to have higher E-factor. Due to lack of innovative green chemistry, the multi-fold production of active pharmaceutical ingredients (APIs) always concomitantly yields exorbitant amount of waste (E-factor: 25-120 kg). In order to get a new drug approved and patented in a competitive pace in a faster manner, quite often, the synthetic route developed turns out to be suboptimal and non-green. Since there is no significant competition to improve patented synthesis before it gets genericized therefore the non-green legacy gets carried forward. Thus, myriad of opportunities arise during innovative research and development of generic APIs towards reducing E-factor and develop cost effective and green synthetic routes for the medicines. Few case studies involving various synthetic strategies to synthesize various APIse.g. Sitagliptin, Naproxen etc.will be presented.



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PL-10

Understanding Rhodopsins through Bioorganic Chemistry

Anil K. Singh

Formerly Professor of Chemistry, Indian Institute of Technology Bombay, Powai, Mumbai – 400 076, India
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Rhodopsins are membrane-bound photoreceptor proteins found in several organisms ranging from bacteria to humans. These photoreceptors are used by the organisms to drive their sensory and energy transductions, including processes as diverse as vertebrate vision to microbial ion transport and phototaxis signaling. Visual pigment Rhodopsin (Rh) is the prime example of such a photoreceptor, and which is the basis of animal vision. Bacteriorhodopsin (bR) found in the purple membrane of *Halobacteriumsalinarium*is another photoreceptor of this type, which allows conversion of light energy into metabolic energy required for vital functions of halobacteria.A great deal of attention has been paid to unravel the structure and function of these photoreceptors, which recently have also received considerable attention because of their potential utility as photoactive element in holographic thin films and memory devices, optical information processing technology, retinal prosthetic devices, colour-sensitive artificial retina,and many other opto-electronic applications.

Our endeavor over the years has been to gain molecular insight into the structural and functionalmechanismsof these photoreceptors through bioorganic approaches, and further utilize the knowledge gained to design their functional analogues and variants.This talk, will elaborate upon how bioorganic models of Rh and bRwere designed and used for developing a molecular understanding of the general structural and functional features of these photoreceptors. The photoactive element of these photoreceptors consist of a specific isomer of vitamin A aldehyde (retinal) covalently linked *via* a Schiff base linkage to the ε-amino group of a lysine residue of a surrounding protein.In spite of the diversity of occurrence in wide range of hosts, these photoreceptors use a common ultrafast photoisomerization of their retinylidene Schiff base chromophore to store/transfer light energy, which ultimately is employed to drive protein's function *via* complex protein-chromophore interactions. The nature of protein-chromopphore interactions, the colour-control mechanism, the nature of excited state of retinyledene Schiff base chromophore, and the protocols of design and development of functional analogues and variants of bR will be discussed in detail. Also will be highlighted design and development ofsynthetic single-cycle photoswitches as one-dimensional caging platforms for spatially and temporally-controlled photorelease of bioactive compounds under physiological conditions, andmultiple-cycle photoswitches,capable of controlling structure and functions of proteins and enzymes.

It is also of value to mention that despite numerous multi-disciplinary efforts made for the past several decades tobuild and understand the structure and mechanism of functionsof these photoreceptors, several questions stillremain unanswered.For instance, the excited state structure and dynamics of the chromophore and its photophysical behavior, the structural features of the photo-intermediates, and development of practical opto-electronic devices based on these photoreceptors, etc. are still a matter of discussion and debate, and actively pursued object of research.Truly, the Rhodopsins present challenge and indeed an unique opportunity to chemists and biologists for not only unraveling the basic principles underlying their functioning but also for developing efficient analogues and variants for various purposes. The coming years are expected to witness continued and enhanced efforts in these areas. This talk, while focusing on our efforts, will also review the recent accomplishments in the field and highlight future inroads into other fields.

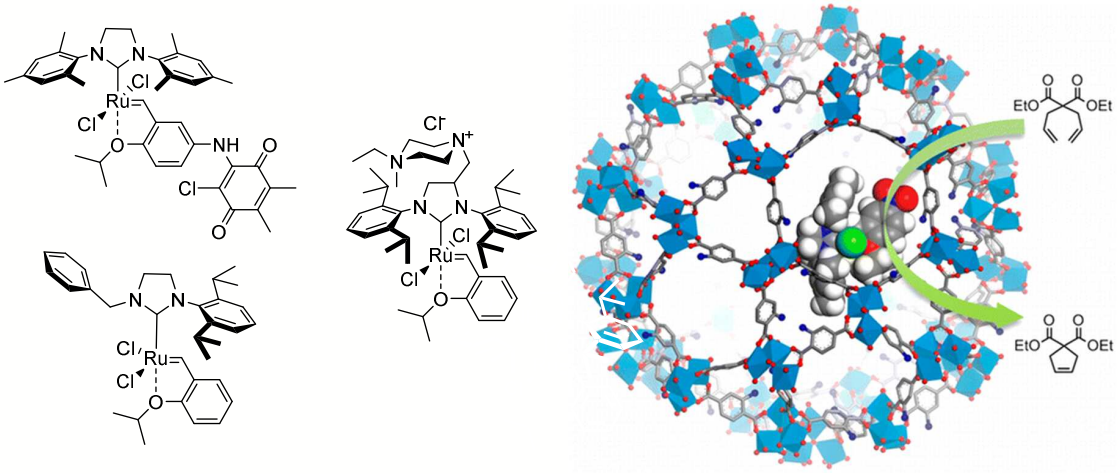
PL-11

MACROCYCLISATION AT HIGH CONCENTRATION AND OTHER PROBLEMS OLEFINMETATHESIS: LOOKING FOR SOLUTIONS

Anna Kajetanowicz

Biological and Chemical Research Centre, Faculty of Chemistry, University of Warsaw, Żwirkii Wigury Street 101, 02-089Warsaw,Poland
E-mail: *akajetanowicz@cnbc.uw.edu.pl*

Ruthenium-catalysed olefin metathesis reaction is an attractive and powerful transformation for the formation of carbon-carbon double bonds [1]. This methodology is now quite familiar to the most organic chemists as numerous catalysts are available that enable a multitude of olefin metathesis reactions. Although many significant issues associated with this transformation (like *inter alia*: control of *E*/*Z* selectivity [2], the conversion of biomass into valuable products [3], or significant decrease in the content of ruthenium in reaction products [4]) have been already solved, performing the macrocyclisation reactions at high concentration and decreasing the level of isomerisation of double bond, in this and other metathesis reactions, still remains a challenge.



During the lecture out efforts to perform macrocyclization at high concentration will be presented as well as different methods of inhibiting double bond migration. These include (1) the addition of isomerisation inhibitors, (2) the use of specially designed catalysts, (3) the use of catalysts deposited on supports, such as MOFs.

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PL-12

Alok Dhawan

Director, CSIR-Indian Institute of Toxicology Research, Lucknow, India

Abstract Awaited

PL-13

TB Free India by 2025: Roadmap to Prime minister's Dream

Dr Surya Kant

Prof and Head, Department of Respiratory Medicine, King George's Medical University, UP, Lucknow, India
Email: skantpulmed@gmail.com

Abstract: Tuberculosis (TB) and humans have had a long relationship with each other. The relationship has not been a friendly one. For centuries, TB has been a major killer of humans in terms of mortality and morbidity. TB is the leading infectious killer in India. It is the first time in medical history that our Honorable Prime Minister decided the roadmap to eliminate the TB from India by launching the TB Free India Campaign at 'Delhi End TB Summit'. The government has set a target for complete elimination of TB by 2025, five years before the global target 2030. The government is implementing a national strategic plan (NSP) to end TB by 2025 with huge funding for the next three years to ensure every TB patient has access to quality diagnosis, treatment and support. The new NSP adopts a multi-pronged approach which aims to detect all TB patients with an emphasis on reaching TB patients seeking care from private providers and undiagnosed TB in high-risk populations, treat all patients with a patient-centric approach, prevent emergence of TB in susceptible population groups and build empowered institutions and human resources to streamline implementation. The ministry has formulated the guidance document on nutritional care and support for TB patients which includes guidance on nutritional assessment, counseling and appropriate dietary advice. The programme is also facilitating the TB patients to avail various social support schemes of the state governments. Information Technology (IT) tools for monitoring the programme and treatment adherence is also included. Community engagement is the hallmark and it is becoming a social movement to end TB in India. Under the Revised National Tuberculosis Control Programme, the government has also proposed an incentive of Rs.500 per patient per month for the nutritional support of TB-affected patients during the course of the treatment.

Keywords: Tuberculosis, National Strategic Plan, Information Technology, Revised National Tuberculosis Control Programme

PL-14

NMR in Chemistry, Biology, Health Sciences and beyond.

C.L. KHETRAPAL

Centre of Biomedical Magnetic Resonance, Sanjay Gandhi PGI Campus, Lucknow

Nuclear Magnetic Resonance (NMR) as a noninvasive technique for studying structure and function of molecules has been in use ever since the discovery of the phenomenon about 7 decades back. However, today it has become an interdisciplinary science which not only integrates physical, chemical, biological and medical sciences but it goes even beyond. Besides understanding molecular structure and function, it is extensively employed to investigate fundamental changes of diseases at molecular level, and to develop molecular interventional methodologies to control and cure them. Its importance was realized only after 1970s when many new techniques in NMR, MRI, MRS and many others were developed. This discipline bridges the contemporary medical and basic sciences. In recent years it extends even beyond to integrate psychological processes, human behavior and spirituality! This is because of new developments in techniques and instrumentation. However, developments of innovative techniques for understanding human diseases at molecular level are still at infancy although enormous efforts are being made in this direction. Monitoring the changes in dysfunctions at molecular level is more sensitive in identifying diseases in early stages giving much room for remedial actions. In addition, understanding human behavior at molecular level provides valuable opportunities of societal relevance. This is the prime objective of this talk and such aspects will be presented with emphasis on our own work.

INVITED

IL-1

Fascinating Adventures in Development of a Drug from Conception to Commercialization: A Personal Perspective

Mukund S. Chorghade

While biotechnological advances, genomics and high throughput screenings or combinatorial and asymmetric syntheses have opened new vistas in drug discovery, the industry is facing a serious innovation deficit regarding discovery and development of NCEs. The current and conventional practices of discovery and development are plagued with high failure rates, long time lines, high cost, poor quality of chemical series:

- High throughput synthesis and combinatorial chemistry produce libraries of flat and planar molecules devoid of chirality and scaffold diversity
- Novel target and concepts have high failure rates in achieving therapeutic outcomes to serve unmet clinical needs
- Conventional practice of one target / one molecule frequently achieves efficacy only in a small number of patients, particularly for indications for etiology involves multiple factors

We pursued an unconventional strategy of leveraging the ancient practice of traditional Indian medicine for discovering and developing Pharma and agrochemical candidates with high success rate, speed and cost-effectiveness. The starting point is a chemical series identified with a proven track record for efficacy and safety. Modern science including bioinformatics tools have been leveraged to identify novel chemotype(s) for lead optimization, for identification of mechanism of action as well as for establishing proof of concept in animal models. We began our search based on clinical experiences, observations or available data on actual use in patients as a starting point. Since safety of the materials is already established, we undertook pharmaceutical development in parallel to controlled clinical studies. Drug discovery follows a 'Reverse Pharmacology' path from Clinics to Laboratories. We describe such approaches with selected synthesis methodologies implemented by us.

We report advances in proprietary in vitro green chemistry-based technology, mimicking in vivo metabolism of several chemical entities used in pharmaceuticals, cosmetics, and agrochemicals. Our catalysts enable prediction of metabolism patterns with soft-spot analysis Metabolites are implicated in adverse drug reactions and are the subject of intense scrutiny in drug R&D. Present-day processes involving animal studies are expensive, labor-intensive and chemically inconclusive. Our catalysts (azamacrocycles) are sterically protected and electronically activated, providing speed, stability and scalability. We predict structures of metabolites, prepare them on a large scale by oxidation, and elucidate chemical structures. Comprehensive safety evaluation enables researchers to conduct more complete in vitro metabolism studies, confirm structure and generate quantitative measures of toxicity.

IL-2

Natural Product-inspired Green Chemistry Approach for the Synthesis of Polyphenolic Compounds of Biological and Industrial Relevance

Arun K. Sinha*

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Polyphenols are naturally occurring compounds found largely in the fruits, vegetables, cereals and beverages. Fruits like grapes, apple, pear, cherries and berries contains up to 200–300 mg polyphenols per 100 grams fresh weight. Typically a glass of red wine or a cup of tea or coffee contains about 100 mg polyphenols. Cereals, dry legumes and chocolate also contribute to the polyphenolic intake.Polyphenols are secondary metabolites of plants and are generally involved in defense against ultraviolet radiation or aggression by pathogens.Thus, the discovery of biologically active polyphenolic natural products including hydroxylatedstilbenes,chalcones andstyreneshas proven to be a subject of considerable importance in chemistry and medicine. Interest in accessing these polyphenolics have gained pace because of plethora of biological activities such as anticancer, antibacterial, antifungal, anti-inflammatory and antimalarial etc. However, exploration of these phenolics is severely hindered by their insufficient percentage in their natural resources, difficult isolation procedure, limiting trials for wider applications besides their tedious synthesis involving protection-deprotectionstrategy. A protection/deprotection event introduces at least two steps into a sequence, incurring costs from additional reagents and waste disposal besides leading to a reduced overall yield. In this context, the concept of Green Chemistry has provided a fresh stimulus to develop a strategy with minimum number of steps, atom economy and waste minimization besides being devoid of protection-deprotection steps. For this various tools and strategies of green chemistry such as microwave-assisted reactions, ionic liquid, tandem reactions, cooperative catalysts, biocatalyst, water-assisted reaction etc are being explored for the synthesis of various bioactive small molecules including phenolic and thiophenoliccompounds. Our group from noticeable time working on such green methodologies for synthesis of various phenolic based bioactive molecules like FEMA-GRAS approved 4-vinylphenols, stilbenoids (symmetrical/unsymmetrical, distyrylbenzene and octupolar stilbenes) andstilbene-chalcones/stilbene-cinnamate hybrids and their biological evaluation. The details will be discussed during presentation.

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IL-3

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Abstract Awaited

IL-4

An efficient one-pot multicomponent synthesis of Diverse Heterocyclic Scaffolds and their Biological importance

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Abstract: The sequencing of multicomponent reactions (MCRs) and consequent cyclization reactions is an influential trick for the quick synthesis of diverse heterocyclic scaffolds. The most advantageous MCRs is adequately flexible that it can be working to produce adducts bearing a diversity of functional groups that may then be selectively balancing to enable different cyclization manifolds, thus most important to a diverse collection of Pyridine, dihydropyridine,Pyrimidone and pyrazolodihydropyridine derivatives. The growing interest in diversity-oriented synthesis with these derivatives has led to increased attention towards the Biological as well as medicinal importance and inspired many advances in the design and implementation of MCRs for the construction of diverse heterocyclic scaffolds.

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IL-5

Carbocyclic derived analogs: A promising scaffold towards discovery of antiviral drug like nucleoside.

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Abstract: The nucleoside class of molecules shown promisingtherapeutic agents as anticancer and antiviral agents. Further, it has its own drug like limitation such as poor selectivity, off-target activity, stability, followed by drug toxicity. It is well documented that carbocyclic nucleoside may provide excellent alternative of nucleoside with enhanced drug like profile.

Entecavir, a carbocyclic nucleoside analog, is the most potent inhibitor of HBV replication on the market.Aristeromycin and Neplanocin are known for their wide range of antiviral activities. Nucleosides substituted at 4'-have attracted attention as festinavir (anti-HIV) and balapiravir (anti-HCV) reached a later phase of development.However, due to limited synthetic methodologies,carbocyclic nucleosides have little representation in the literature. Owing to the importance of carbocyclic as antivirals, we aim to combine theirstructural features including to generate several new analogs and antiviral evaluation.

In continuation structure-based approachand molecular modeling provided a directionfor new scaffold synthesis using base and pseudo sugar modification to get selective antivirals. The combined studies suggest the discovery of promising molecules based on carbocyclic nucleoside with new mechanism of action. (Authors thanks to DST, India for financial support.)

IL-6

Efficient Syntheses of Drug-like Nitrogen Heterocycles

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Nitrogen heterocycles are among the privileged motifs that play vital roles in natural products and therapeutic agents endowed with antiproliferative activities. Identification of new chemotherapeutic agents for the treatment of cancer affliction is one of the leading areas in drug discovery (1). Most of the anticancer agents are found to possess undesirable actions such as toxicity, reduced bioavailability and drug resistance. Therefore, hunt for potent and selective anticancer agents are highly encouraged. In line with this pursuit we have been investigating potent anti-proliferative agents containing indole, carbazole and porphyrin units. Developing mild, economical and scalable synthetic strategies to access valuable heterocycle-based agents are enduring challenges and immense scope for organic chemists. Our efforts to prepare bioactive heterocycles involve synthetic strategies like C-H functionalization, oxidative cyclization, click chemistry and metal-free direct arylation. Recently, we have demonstrated the synthetic utilities of organoiodine reagents to access 2-arylindoles, heteroaryl carboxylates, *N(O)*-arylquinolones, fused triazoles, oxazoles, oxadiazoles, thiadiazoles, natural products (Pallulone and Glycosinine) and drug analogues of Tafamidis and Boscalid (2). Recent strategies to access drug-like heterocyclic molecules will be presented in the presentation.

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IL-7

Searching a target to treat metabolic syndrome: Brown fat or the muscle?

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Metabolic syndromes including obesity and type II diabetes are becoming more and more common all over the world. It is widely accepted that this trend is due to dysregulation in the energy homeostasis of an individual. In an animal body, energy enters in the form of food and exits as work and heat. The body tries to store the unspent energy and this activates several metabolic remodeling of various organs, which is a major cause of initiating the program leading to the metabolic disorders. However, mammalians have ability to resist excessive weight gain due to energy surplus which has been termed as “Diet Induced Thermogenesis or DIT”. Ever since the discovery of DIT in 1970s, researchers have been focusing to delineate mechanisms that contribute to this process. Early studies established the role of uncoupling protein 1 (UCP1) in the inner mitochondrial membrane of brown adipose tissue (BAT) in DIT. BAT is the major organ of cold-induced nonshivering thermogenesis (NST) in eutherian mammals. We have shown that the other site of NST in mammals, the skeletal muscle, is also activated during both cold and DIT. Recently, a third mechanism called “beiging” has been proposed to be involved in DIT, which can be based on either UCP1 dependent or independent processes. Now, there is a hot debate in the field as to which of these three mechanisms of DIT can be the best to target pharmacologically for countering obesity (and/or diabetes) in humans. Targeting mitochondria for obesity brings the whole concept into question due to side effects. Muscle NST being based on futile cycling of calcium ions and not on mitochondria directly, seems to be a safer route to increase energy expenditure and reduce energy surplus thereby countering obesity. Therefore, it is necessary to carefully define the details of mechanism involved in activation and maintenance of muscle NST.

IL-8

New frontiers in gas-phase cavity ring-down spectroscopy for medical diagnosis and environmental sensing

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Cavity ring-down spectroscopy (CRDS), an optical cavity-enhanced absorption technique, directly measures the rate of absorption of light in place of the magnitude of absorption when the light is circulating in a high-finesse optical cavity. Because of its unique approaches, the ring-down technique readily offers 10 to 100 million times better detection sensitivity when it is compared with the traditional absorption spectroscopy techniques.

In this talk, I will discuss our latest developments of new-generation gas-phase ring-down spectroscopy techniques combined with the cutting-edge external-cavity quantum cascade lasers (EC-QCLs) operating in the mid-IR molecular fingerprint region [1,2,3]. I will talk about high-resolution fundamental molecular spectroscopy of numerous atmospherically and bio-medically relevant important molecules and their isotopic species such as $^{12}CH_4$, $^{13}CH_4$, $H_2{}^{32}S$, $H_2{}^{33}S$, $H_2{}^{34}S$, NH_3, N_2O, NO and C_2H_2 exploiting the EC-QCL-based high-precision *cw*-CRDS technique. I will also talk about their ultra-sensitive detection and quantifications in a variety of environments such as in ambient air as well as in human exhaled breath with unprecedented sensitivity (in parts per billion, ppbv to parts per trillion, pptv levels) and high molecular selectivity.

Then, I will talk about how fundamental gas-phase CRDS spectroscopy can be employed in real-life applications in healthcare environments for *non-invasive* molecular diagnosis of diseases. I will particularly talk about our innovations and technology on the development of prototype breath analyzer [4] exploiting gas-phase spectrometry, which can precisely and selectively diagnose stomach infection and ulcer disease by analyzing some unique panels of molecular species in human breath. The spectroscopic signature of the breath molecules, so called “breath-print” and the new prototype system will obviate painful endoscopy-based biopsy tests. The new device is now under the clinical validation in a hospital environment as a prelude to technology transfer and subsequent commercialization. Finally, I will talk about some potential future directions of our work on gas-phase ring-down spectroscopy where new technology and products could be developed for societal applications.

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IL-9

Applications of LC- MS tools in natural products

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Abstract: Herbal medicines and their preparations have been widely used for hundreds of years all over the world. The efficiencies of herbal medicines depend on the amount of active components in them, which could vary significantly in contents. Therefore, the discovery of relevant metabolites and fingerprints allow the introduction of an appropriate QA/QC in Traditional medicine. It is a most demanded area and an essential requirement to improve our traditional knowledge of herbal medicines. This presentation involves the use of hyphenated mass spectrometricmethods such as HPLC/ESI-QTOF-MS/MS and UPLC-MS/MS and DART-MS for qualitative and quantitative analysis of bioactive constituents in selected medicinal plants. It also describes the methods for mass fingerprinting. Phytochemical markers were identified for quality control and authentications of plants/parts and their products.

Keywords: Herbal medicines; Hyphenated mass spectrometric methods; mass fingerprinting

IL-10

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Abstract Awaited

IL-11

Privileged Scaffold Diversification through C–H bond functionalization using 1st Row Transition Metals-catalysts

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The stark impediment to carry out the chemistry for the formation C–C and C–X bonds is the requirement of pre-functionalized expensive substrates which, indeed, are in demand of multistep synthetic protocols to prepare. In addition, formation of stoichiometric amounts of bi-products (mostly halide salts) also serves as the major restraint for the economic and environmentally benign synthesis of substrates of requirement as pharmaceuticals or materials. Therefore, although extremely challenging, thermodynamically and kinetically disfavoured direct C–H functionalization of hydrocarbons using transition-metal catalysts has been the latest efforts, offering straightforward synthesis of substrates with high atom economy. In this endeavor, various transition metal-catalyzed conditions have been established. However, in general, 2nd and 3rd row transition metals have been used very frequently, despite being known for their high cost and handling problem, moisture and air sensitive (require glove box), hazardous and toxic nature. On the other hand, low cost, air stable and easy to handle 1st row transition metal-catalysts were not employed very frequently for the direct C–H functionalization. The obvious reason could be the less reactivity of these catalysts in terms of C–H metalation. However, if tuned properly, either the directing groups, or ligands, these catalysts would be capable to induce C–H functionalization.

In the presentation, we will be discussing our recent endeavor to activate C–H bond using catalysts based on 1st row transition metals.

IL-12

Tips for Effective Preparion of Scientific Reviews

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Successful production of a written product for submission to a peer?reviewed scientific journal requiressubstantial effort. Such an effort can be maximized by following a few simple suggestions when composing/creating the product for submission. Writing for publication can be a challenging yet satisfying endeavor. The ability to examine, relate, and interlink evidence, as well as to provide a peer?reviewed, disseminated product of your research labors can be rewarding.

Publishing scientific review article in the prestigious journal is a great challenge for the research community. The preparation of a draft (proposal) for initial submission to the journal editor for acceptance and further permission for writing a full manuscript will be discussed. Before preparation of manuscript, construction of review article and technical steps, viz.; title of article, authorship-affiliation, abstract, introduction, main text, conclusion/summary/future perspectives, acknowledgement, abbreviations, references and biography of author(s) will be discussed. After submission of full article to the journal, the different steps before the final acceptance and later too will be shared. A few suggestions may offer in this presentation that may assist the novice or the developing writer to attempt, polish, and perfect their approach to scholarly writing.

IL-13

Linear dicarbonyls as suitable substrates for amine catalyzed transformations: Synthesis of medium-sized *N*-heterocyclic compounds

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Organocatalysis has grown-up rapidly and applied successfully to several different enantioselective reactions in last one decade and therefore, now considered as the "*third pillar*" of enantioselective catalysis, together with biocatalysis and metal catalysis.[1] Additionally, nitrogen heterocycles constitutes a number of small molecule natural products (SMNPs) acts as therapeutic agents for the treatment of a plethora of diseases that confront humankind in an age where the rapid emergence of multi-drug resistant forms are becoming an increasing threat. In the continuation of our interests,[2] recently we have developed new methods for the asymmetric and non-asymmetric synthesis of medium sized nitrogen heterocycles targeting SMNPs using aminocatalyzed transformation of dicarbonyls through donor-acceptor (D-A) annulation approaches. Details of the D-A concept, design and synthetic strategy for medium sized nitrogen heterocycles using glutaraldehyde will be presented here.

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IL-14

A simple synthesis of transition metal nanocrystalline ferrite:An effective and environmentally benign catalystfor the one-pot multicomponentreactions.

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Abstract: Recent applications of transition metal nanocrystalline ferrite as catalyst in organic synthesis performed through multicomponent reactions is an attractive area of research and most important processes for the preparation of highly functionalized organic compounds.Transition metal nanoferritescatalyst addresses the sustainability concerns and provides alternative efficient methods for various important organic transformationsin the field of heterogeneous catalyst. The transition metal nanocrystalline soft ferrite [MFe_2O_4, M (II) = Mg, Cu, Co, Ni and Zn] prepared by co-precipitation method and hard hexaferrite using solution combustion method. The synthesized materials were characterized by thermal analysis, powders X-Ray diffraction, SEM, and FTIR analysis for evaluating phase, structure and morphology and stoichiometry.To know the magnetic hysteresis interactions, the magnetic measurements were carried out at room temperature by using SQUID Magnetometer with a maximum applied field of ± 5 T.The catalytic performance of metal spinel ferrite nanoparticles towards the synthesis of 2-3 dihydroquanozolin 4(1*H*) one,3,4-dihydropyrimidin-2(1*H*)-ones/thiones Hantzch 1,4-dihydropyridine, tetrahydrodipyrazolopyridine and benzoxazin-ones/thiones derivatives with varied substitution have been described.This protocol offers several advantages including its greenness with respect to mild reaction conditions, good yields of products, short reaction time and operational simplicity. The catalysts retain their activity and product yield up to four cycles.The formation of compounds were confirmed by using FT-IR, ^{1}H &^{13}C NMR spectralanalyses and compared with reported values.Based on our findings, a plausible mechanism involved in the catalytic reaction is also proposed.

IL-15

Imidates: A Versatile Synthons for Organic Chemists

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Abstract: Functionalized organic molecules are an important class of compounds that are ubiquitously present as a structural motif in natural products, biologically active compounds, and in several physiologically active agents such as nucleic acids, antibiotics, hormones, *etc*. The synthesis of the highly functionalized organic molecules, particularly α-ketoamides, α–oxoesters, diaryl 1,2 diketones, α–amino esters and α–acryloxy esters derivatives, are high in demand not only for the construction of natural products but also in asymmetric syntheses, agrochemicals, and material science.[1,2]

Imidate (also known as imino ether) is considered as one of the most important and versatile moiety among the various functional groups in organic chemistry. In the recent time imidate moiety has been extensively employed in synthetic and medicinal chemistry because of their unique electronic features and importantly serve as potent electrophiles in contrast to the corresponding amides and carbonyl functionality. Considering the interesting chemistry and high importance, we became interested in exploring the chemistry of imidate for the synthesis of high value-added derivatives of organic compounds.[3] The scope and limitations of such chemistry will be discussed using selected examples.

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IL-16

Dienophilicity of >C=P– Functionality of 2-Phosphaindolizines towards Electron Rich Vs Electron Deficient Dienes

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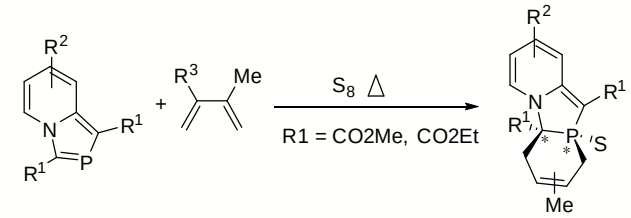
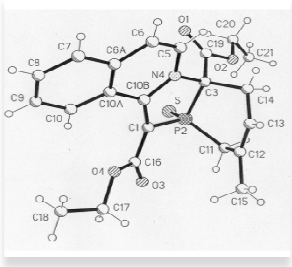
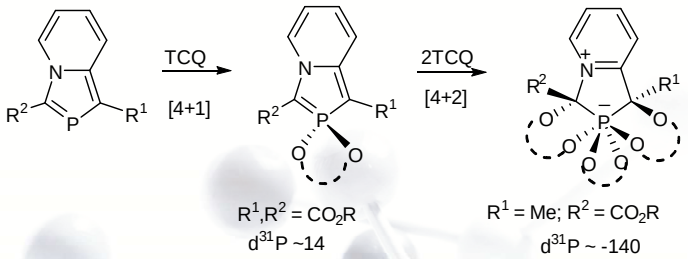
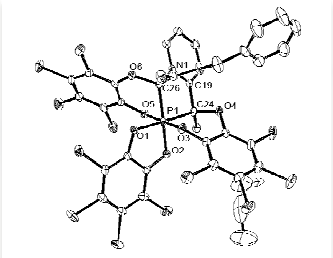
Reactivity of the >C=P– functionality of 2-phosphaindolizines towards Diels-Alder reaction with 1,3-dienes has been found to be dependent on the substituents on the two carbons adjacent to the phosphorus atom of the azaphosphole ring as well as nature of diene electron rich or electron deficient. 1,3-Bis(alkoxycarbonyl)-2-phosphaindolizines undergo diastereoselective Diels-Alder reactions with 2,3-dimethylbutadiene and with isoprene at the >C=P- functionality in the presence of sulfur. Observed 100% regioselectivity in the reaction with isoprene has been rationalized on the basis of DFT calculations. The relative stabilities of the transition structures have been explained on the basis of the NBO analyses. Reactivity of electron deficient heterodiene orthoquinones towards 2-phosphaindolizines has also been found to be substituent dependent. In the presence of EWG on two adjacent carbons to phosphorus, only 1:1 cheletropic [1+4] cycloadduct was formed. Recently, a novel polycyclic hexacoordinate zwitterionic phosphorus heterocycle resulting from tandem sequential [1+4] and double [2+4] cycloadditions on >C=P– functionality of 2-phosphaindolizine in the absence of an EWG at 1-position has been obtained and charachterized. Effect of the EWGs on control of the reaction sequence by the nature of HOMO has been investigated computationally.









IL-17

Development of Chiral Catalysts for Asymmetric Aldol and Henry Reactions

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Abstract: The enantioenriched compounds have various applications including pharmaceuticals, agricultural chemicals, flavours, fragrances and material.[1,2] Asymmetric catalysis is defined as an enantioselective transformation controlled by a chiral catalyst. We are working on the development of organocatalyst as well as chiral metal complexes for asymmetric organic transformations. We have developed variety of catalyst having(*L*)-Prolinamides is catalytic active unit which were synthesized from *trans*-4-hydroxy-(*S*)-proline or (*S*)-proline and chiral/achiral amines (Figure 1).These prolinamides were evaluated for the asymmetric aldol reaction between 4-nitrobenzaldehyde and cyclohexanone, afforded product in excellent yield and 95% *ee* with *anti:syn* (88:12) after 18 h.The catalyst **7** can be used up to 5 continuous cycles for asymmetric aldol reaction between 4-nitrobenzaldehyde and cyclohexanone with overall 91% yield and 86% yield of *anti*-product with *anti:syn* (98:2).[3] We also applied these catalysts for the asymmetric aldol reaction between isatin and acetone.[4]

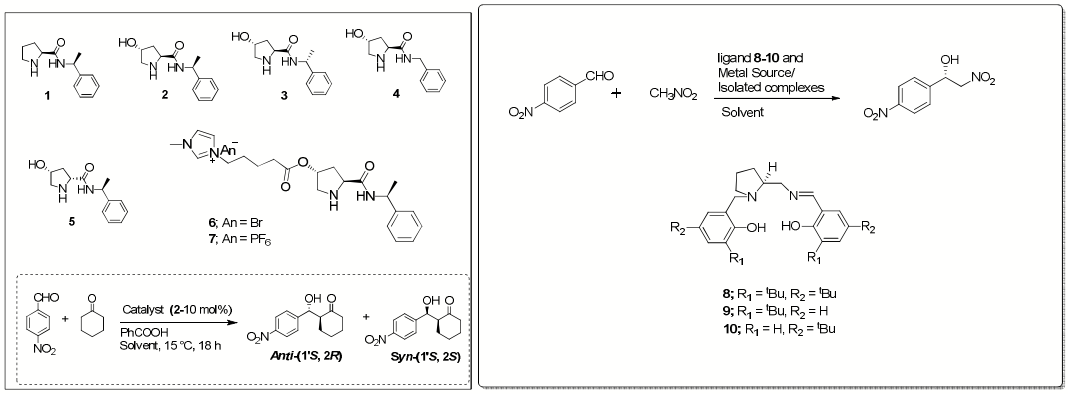

Figure 1: Asymmetric Aldol reaction and Henry reaction

We have also developedsingle chiral center C_1 symmetric salalen ligands(**8-10**) were synthesized from (*S*)-proline and its Cu(II) and Mn(III) complexes were used as catalysts for the asymmetric Henry reaction between aromatic aldehydes and nitromethane/nitroethane.[6]

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IL-18

The triple role of 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU) in the synthesis of diaryl ethynes and enynes from 1,1-dibromoalkenes at ambient temperature

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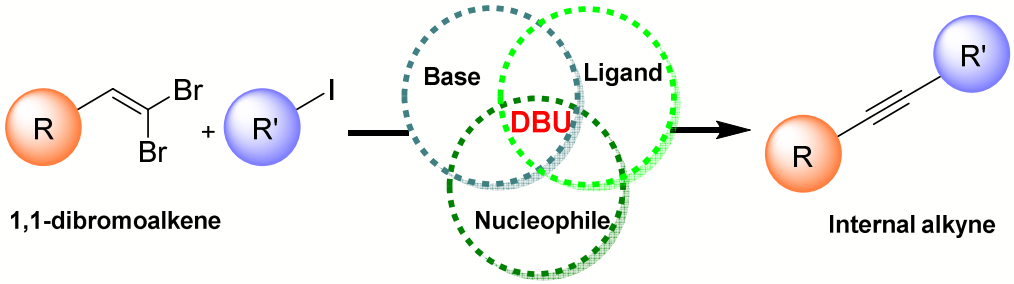
Abstract: The unique method presented herein features a bicyclic amidine that serves three distinct mechanistic functions, *i.e.*, serving as a base, nucleophile and ligand, in this synthetic transformation. The reaction of 1,1-dibromoalkenes with DBU in the presence of a Pd(II)/Cu(I) catalytic system afforded diaryl alkynes and enynes at ambient temperature. Control experiments demonstrated the essential role of DBU in this transformation. The unusual stability of the key catalyst, $Pd^{(0)}(DBU)_2$, allowed it to be characterized by HRMS analysis.



● *Substrate scope on either side* ● *Ambient temperature* ● *34 examples*

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IL-19

Myoglobin-catalyzed olefin-cyclopropanation reaction

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Olefin cyclopropanation is a particularly valuable transformation owing to the occurrence of cyclopropyl moieties in many bioactive natural and synthetic compounds. A well-established chemical approach to olefin cyclopropanation involves transition-metal-catalyzed decomposition of diazo reagents followed by metallocarbenoid insertion into C=C bonds. A wide range of transition-metal complexes have demonstrated utility in this respect, with the use of chiral ligands enabling these reactions to proceed in an asymmetric manner. Despite this progress, achieving high levels of both diastero- and enantioselectivity, also in combination with high catalytic activity, remained a significant challenge in these processes. This work reported the successful design and application of myoglobin-based cyclopropanation biocatalysts that are capable of offering high *trans*-selectivity along with complementary stereoselectivity across a broad panel of aryl-substituted olefins [1].
Furthermore, these myoglobin-mediated transformations can be performed in the context of whole-cell systems, which further simplifies their use for synthetic applications. The biocatalytic systems developed here have enabled the stereoselective synthesis of multiple cyclopropane-containing drugs at the preparative scale, offering superior performance over currently available methods for asymmetric cyclopropanation or granting a more concise route to their preparation [2].

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IL-20

Newer Trends of Drug Discovery: Current Status of Nitric Oxide Synthase (NOS) Inhibitors

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The drug discovery is a core area in the pharmaindustry for developing new drugs, and it is as such very lengthy process and quite challenging with various new diseases.However, the pharma industry is heavily invested on the new drug discovery and development of New Chemical Entities (NCEs) based on the disease targets, but the speed of drug discovery process is driving factor to launch new inventions to the market. Apart from traditional medicinal chemistry, several newer drug discovery approaches are developed including DNA-encoded chemical libraries and others.The main objective(s) of the each approach could enhance the speed of the process and develop safer medicines.Most significant disease targets are based on the enzymes, and enzymology will play significant role to explore new innovations in the drug discovery.

Nitric oxide synthase (NOS) is an oxidoreductase enzyme catalyzes the conversion from L-arginine to L-citrulline and nitric oxide (NO) by three highly distant isoforms of nitric oxide synthases (NOSs), namely neuronal (nNOS), inducible (iNOS), and endothelial (eNOS). All three NOS isoforms generates nitric oxide (NO) from L-Arginine through an oxidation process involved with molecular oxygen and NADPH. Nitric oxide (NO) has various physiological roles including vascular tone in endothelial system, host-defense in immune system, and long-term potentiation and memory in neuronal system. However, NO is involved with number of pathophysiological conditions due to high or low levels, and most notably stroke, migraine, septic shock, arthritis, and multiple sclerosis. Therefore, considerable efforts are focused in the development of NOS inhibitors and designing such inhibitors based on amino acid and non-amino acid type small molecules. In the presentation, design, synthesis, and biological activity of various small-molecules based on the structural motif of isothioureaand others for the inhibition of NOS isoforms will be discussed.

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IL-21

Myoglobin Reconstitutedwith Manganese Porphycene – A Promising Bio-catalyst for C-H Activation: An insight into the Theoretical Investigation

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Wild type myoglobin usually works as oxygen storage protein and it has no peroxygenase or oxygenase activity though it possesses the same heme prosthetic group as cytochrome P450. It is one of the accepted challenges taken by the scientist to make it a catalyst for C-H with the help of enzyme engineering. A successful effort was done by Hayashi and his co-worker [1]. They have found that the myoglobin can be a promising catalyst if it is reconstituted with Mn-Porphycene. But there are so many questions need to be addressed to understand the mechanistic insights properly and for further progress. Why reconstituted Mn-porphyrin is reactive? Finally, what is the role of protein matrix as free Mn-porphycene also not works as C-H activation catalyst? A rigorous theoretical investigation has been performed to clarify all the aforementioned issues and will be presented in this lecture [2].

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IL-22

Coupling slow H_2S donors with drug fragments: A new strategy in discovering low toxicity drugs.

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Abstract: H_2S is a Gasotransmitter like NO and CO which have bimodal physiological effects. At low concentrations it induces anti-inflammatory and cyctoprotective signaling, while at higher concentrations it induces apoptotic effects. The pharmacological effects of H_2S depend not only on its concentrations but also on its rate of generation. This was also the reason for lot of discrepancies existing in initial literature about its biological effects. Recently, slow H_2S donors were found active as anticancer, antihypertensive and anti-inflammatory agents. Herein, we want to report some findings from our lab, in perspective with findings from other groups that hybridization of slow H_2S donors with in vivo active anti-leishmanial molecule resulted in an anti-leishmanial agent which killed intracellular amastigotes without even deforming host macrophages.

Reference:

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IL-23

Identification of lead antimalarial and anti-Parkinson molecule *via* molecular hybridization approach

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The design of new molecules with improved ADME properties along with effective pharmacological potency; lack of toxicity and devoid of resistance for the treatment of infectious diseases has remained a big challenge for the scientific community. In order to address these issues concept of molecular hybridization was put forward wherein two or more distinct pharmacophoresare covalently linked into a single molecule that may lead to a molecule with improved efficacy [1]. This approach may solve the problem of drug resistance and reduce the undesired side effects [2]. The development of such molecular frameworks with synthetic selectivity and economic viability is still a challenging task for the pharmaceutical industry. Drugs developed through this approach can be used for the cure of infectious diseases where treatment is limited to few drugs and the known drugs have limitations such as toxicity, pharmacokinetics, pharmacodynamic and drug resistance. The benefit of using molecular hybrid is to activate different or same targets by a single molecule, and increase the therapeutic efficacy and to improve the bioavailability. Molecular hybridization approach has resulted many drug candidates with improved activity profile and some of these compounds are in clinical trials. Towards these goals we have synthesized various molecular hybrids and tested these for antimalarial, anti-TB and anti-cancer activities and efforts will be made to present our recent work [3-19].

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IL-24

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Plant Biotechnology Products:Bio-safety and health security

IL-25

ANTI-INFLAMMATORY EXPLORATION OF SULFONAMIDE CONTAINING DIARYL PYRAZOLES WITH PROMISING COX-2 SELECTIVITY AND ENHANCED GASTRIC SAFETY PROFILE

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ABSTRACT :

Objectives: Novel sulfonamide containing diaryl pyrazoles were synthesized and were screened for anti-inflammatory studies.

Methods: All the newly synthesized derivatives were ensured by spectral and elemental analysis and were subsequently tested for their *in-vitro* cyclooxygenase inhibitory assay. Compounds that showed promising *in-vitro* COX-2 IC_{50} values and selectivity indices were then evaluated for their *in-vivo* anti-inflammatory inhibition assay using standard carrageenan induced rat paw edema method. Two promising inhibitors were evaluated for ulcerogenic liability. X-ray crystal structure of COX-2 was taken from PDB entry COX-2 (3LN1) having resolution of 2.80 Å (Angstroms). Structural preparations for docking studies were accomplished using protein preparation wizard in Maestro 9.0.

Results: Compounds **10b** displayed reasonable COX-2 inhibition (COX-2 IC_{50}=0.52 μM) and COX-2 selectivity index (SI=10.73) when compared to Celecoxib (COX-2 IC_{50}=0.78 μM) and (SI=9.51). In-vivo anti-inflammatory studies demonstrated 64.28% inhibition for **10b** in comparison with the 57.14% for that of Celecoxib itself. The results of ulcerogenic liability were also found comparable with standard celecoxib. Molecular docking studies revealed that, all the designed molecules showed good interactions with receptor active site with glide scores in the range -13.130 to -10.624.

Conclusion: Sulfonamide containing diaryl pyrazoles having admirable anti-inflammatory activities compared to that of standard were prepared.

Keywords: Diaryl pyrazole, Hydrazide, Sulfonamide, molecular docking, COX-2 Inhibitor, Rat Paw Edema Method, Anti-inflammatory Activity, Ulcerogenicity index

IL-26

Aegeline inspired synthesis of novel β3-AR agonists for insulin resistance and Amino alcohol and thiazolidinedione hybrids for antiadipogenic activity

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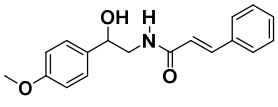
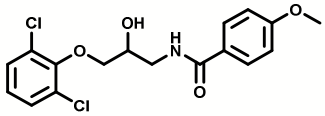
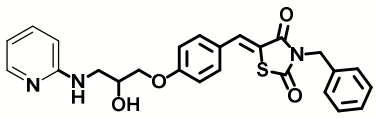
We have reported Aegeline that is N-acylated-1-amino-2- alcohol, which was isolated from the leaves of *Aegle marmelos* showed antihyperglycemic and anti-hyperlipidemic activity for which the QSAR studies predicted the compound to be the β3-AR agonist.[1] As a part of our drug discovery program, we have synthesized and evaluated the β3-AR activity of novel N-acyl-1-amino-3-arylopropanol synthetic mimics of Aegeline and its beneficial effect in insulin resistance. We also synthesized a series of novel amino alcohol and thiazolidinedione hybrid molecules and studied their antiadipogenic activity. The synthesis of Aegeline analogues and their activity results will be discussed.[2-5]



Aegeline





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IL-27

Title: "Method development for C-N bond formation and their applications in medicinal chemistry"

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Abstract: Amines are widely present in various biologically active natural compounds and important intermediates in the preparation of various agrochemicals, pharmaceutical drugs and polymers. Among them, tertiary amines are the most valuable class of chemical compounds, present in natural products, particularly in several biologically active alkaloids, drugs, agrochemicals and widely used in the preparation of surfactants and lubricants. Therefore, the development of novel, efficient and cost-effective catalytic methods for construction of carbon-nitrogen (C-N) bond is a daunting task for the organic chemists. We have developed an Iron-catalyzed strategy for the N-alkylation of arylamines with alcohols *via* a carbocationic pathway. This environmentally amiable, economical catalytic method exhibits a wide substrate scope for the synthesis of various higher arylamines in good to excellent yields. Further, organocatalytic approaches were developed for the mono N-alkylation of anilines using phenylsilane as a reducing agent as well as for the synthesis of tertiary amines from secondary aliphatic and aromatic amines by using economical and environmentally friendly reducing agent. The generality of the organocatalytic method was demonstrated by the N-alkylation of ciprofloxacin and its derivative.

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IL-28

Novel Polymeric Antioxidants and Bio-Antioxidants: Our Extensive Studies

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Over the years, we have studied the anti-oxidant activities of different classes naturally occurring polyphenolic compounds, i.e. coumarins, xanthones, flavonoids, etc. Structure-activity relationships have been drawn and synergistic effects of binary and ternary mixtures of these plant-based antioxidants with well-known antioxidants (DL-α-tocopherol, caffeic acid and L-ascorbic acid) have also been studied.The new binary antioxidant compositions of the studied compounds with DL-α-tocopherol demonstrate higher stability of the lipid substrate than the individual components. All ternary mixtures manifest strong synergism as a result of continuous regeneration of DL-α-tocopherol from both the studied antioxidants and L-ascorbic acid. Reaction schemes for explanation of the new effects observed have been obtained. The role of each component in the antioxidant compositions of ternary mixtures has been identified based on new equations composed by us.

Further, antioxidants are very important additives whose role is to maintain the chemical and physical properties of different materials such as plastics, elastomers, processed foods, lubricants, etc. during transportation, storage, processing and serving conditions. Although conventional antioxidants provide protection against the deleterious effects of reactive free radicals, they suffer from some serious drawbacks such as poor thermal stability, high volatility, poor processability, etc. owing to their molecular size. Various approaches have been followed to make high molecular weight macromolecular antioxidants. These high molecular weight antioxidants have improved extraction and migration resistance and thermal stability and processability, but their antioxidant activity performance suffers greatly. We have designed biocatalytic synthesis of novel polymeric antioxidants and carried out their evaluation for different applications. The polymeric antioxidants thus obtained show remarkably better efficacy and stability.

Results of these co-operative studies between Institutions in India and USA shall be presented at the Conference.

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IL-29

Transition-Metal-Free Approaches for the Synthesis of Heterocycles and Functionalization of sp^3/sp^2 C–H Bonds

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Transition-metal-catalyzed reactions, and especially palladium and copper catalysed reactions, has changed the face of modern organic synthesis.[1] Use of these reactions led to the development of radically new methods of building carbon–carbon and carbon–heteroatom bonds in organic chemistry. However, the drawbacks associated with these reactions such as toxicity, requirement of additional co-catalysts, sensitivity to the air/moisture, need for non-commercial ligands and threshold values in pharmaceutical products serves as inspiration to develop metal-free reactions as an efficient alternative to reactions normally performed by transition-metal catalysis.[1-2] Transition-metal-free reactions display higher efficiency and are often practical, as they are generally less sensitive to air and moisture. Because of the endless pursuit of sustainable chemistry and green chemistry, development of new synthetic strategies under transition-metal-free conditions leading to useful structures remains to be highly appealing and significant. Owing to these facts, we also become interested to explore new approaches for the synthesis of heterocycles and functionalization of sp^3/sp^2 C–H bonds under transition-metal-free conditions (Figure 1).[3-6] The details of the developed methodologies will be discussed.

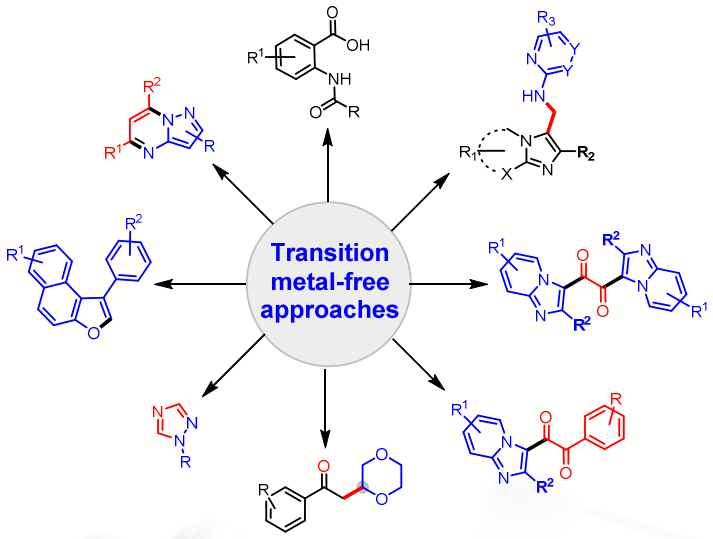

Fig. 1. Transition metal-free synthesis of heterocycles and functionalization of sp^3/sp^2 C–H bonds

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IL-30

Evolution & Interweaving of Diazo Group Chemistry with Visible Light Catalysis

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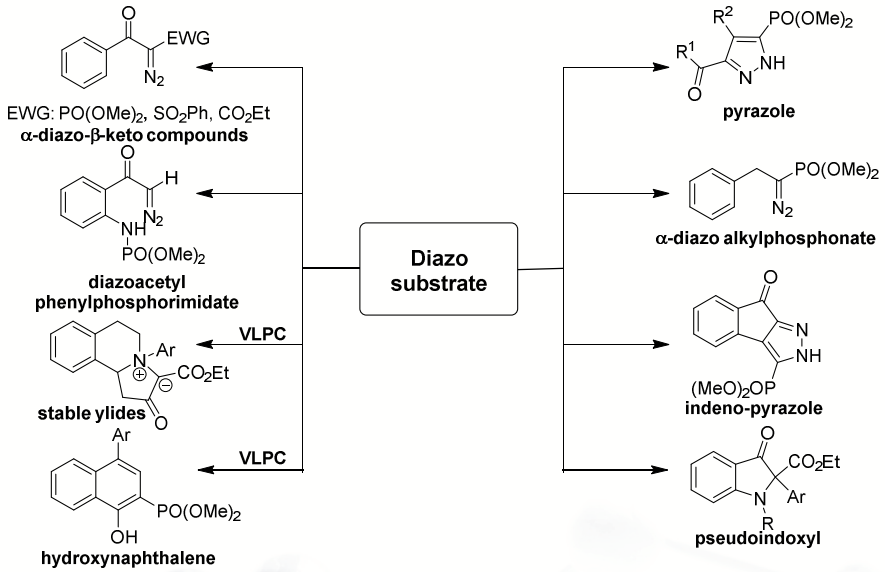
The chemistry of diazo compounds is more than a century old and their unique ambiphilic character makes them valuable building blocks in organic chemistry. They participate as 1,3-dipoles in cycloaddition reactions and owing to their tendency to form carbenes, they participate in Wolff rearrangement, cyclopropanations, insertion reactions, ylide formation and several other useful transformations.[1] Recently, emergence of visible light photoredox catalysis (VLPC) as a greener alternative to the conventional chemical synthesis has led to the development of several useful protocols for C-C as well as C-X (X = halogens, B, O, P, S, Se) bond formations.[2]

Our group developed the synthesis of several valuable scaffolds such as pyrazoles, alkenylphosphonates, α-diazo-β-keto compounds, indenopyrazoles, pseudoindoxyls, hydroxynaphthalenes etc. using diazo compounds as substrates.[3] We also employed diazo compounds in the visible light catalyzed reactions as nucleophiles as well as radical precursors.[4] The talk will highlight the expansion of diazo group chemistry and visible light catalysis in our research group synergistically.



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IL-31

Stereoselective Synthesis of Natural Product Inspired Carbohydridsas Antiproliferative Agents

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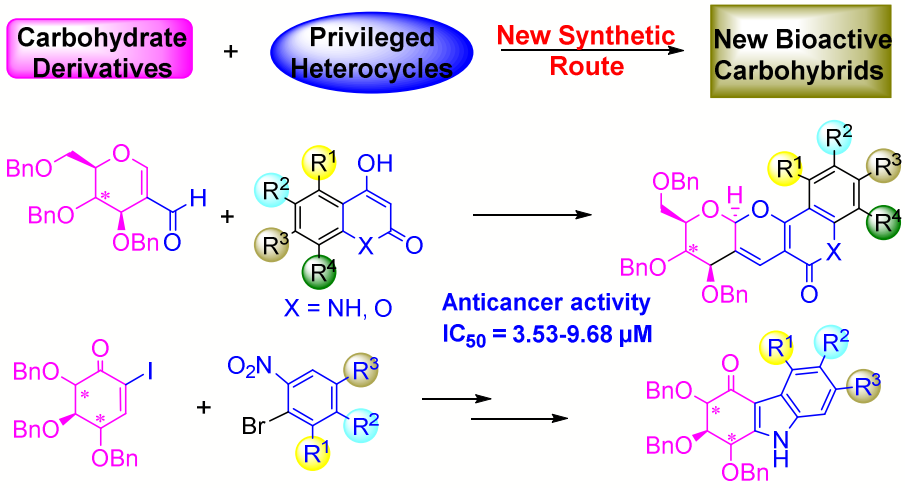

Abstract: Construction of drug like molecules is a challenging task in drug discovery process. Pyrano[3,2-c] -quinolones and -pyranones structural motifs are commonly found in natural products with diverse biological activities. As part of a research programme aimed at developing efficient synthesis of natural products like small molecules, we designed and developed facile stereoselective synthesis of two series of carbohydrate fused pyrano[3,2-c]-quinolone (n = 23) and -pyranone (n = 22) derivatives starting from 2-*C*–formyl galycalsreacting with various 4-hydroxyquinolones and 4-hydroxycoumarins respectively in shorter reaction time (15-20 min). Antiproliferative activity of these synthesized carbohybrids were determined against MCF-7 (breast) and HepG2 (liver) cancer cells. The selected library members displayed low micromolar (3.53-9.68 µM) and selective antiproliferative activity.[1-2]We have also developed a new route for the preparation of chirally enriched tetrahydrocarbazolones and tetrahydrocarbazoles.[3]The details of these findings will be presented therein.

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IL-32

ESIPT based Hydroxy-aryl benzimidazoles/Schiff bases as chromofluorescentsensor and logic devices

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Proton transfer is very fundamental process, occurs in a large variety of chemical reactions as well as in biological systems such as acid-base neutralization and enzymatic reactions. Excited state intramolecular proton transfer (ESIPT) is one studied experimentally and theoretically due to its applications in molecular fluorescence probes, luminescent materials, UV stabilizers, OLEDs and molecular logic gates. In general, the ESIPT process requires hydrogen bond between proton donor (–OH, $–NH_2$, or –NHR etc.) and proton acceptor groups (–C=O, –N= etc.), which must be at interacting distance to each other in a molecule. ESIPT process depends upon the distance of hydrogen bonding i.e. separation between the H-acceptor and donor atoms in molecule. The distance may change depending upon the ring size of system such as 5-membered, 6-membered or 7-membered.

In the present presentation, synthesis of various hydroxyl-aryl benzimidazoles/Schiff baseswill be discussed for exploration of ESIPT phenomenon. These moieties exhibited excited enol and keto tautomeric emission bands.The presence of anions and metal ions has been realized by prohibiting ESIPT through coordination or deprotonation induced by metal and anions with ESIPT centres, resulting in detectable spectral change. Presence of substituent, extended conjugation on ESIPT centres further affects the keto enol tautomerism and thus fine tunes the emission channels. The stimuli induced bathochromic or hypsochromic shift of these normal and ESIPT based emission channels further open new emission channels and thus provided opportunity for simultaneous sensing of multiple analytes, biological interactions, miniaturization of logic gates.

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IL-33

Metal-Free Approaches for the Construction of C-C and C-N Bonds

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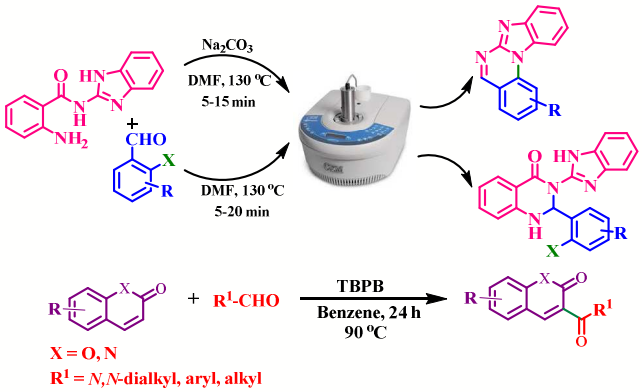
Abstract: Metal-catalysed coupling reactions have proven to be apowerful tool in recent years for the construction of C–C andC–heteroatom bonds through the direct functionalization ofC–H bonds.Although transition-metalcatalysis has become an indispensable tool for direct transformations,it suffers from several limitations, such as the use ofexpensive, toxic and air- and moisture-sensitive catalysts andexpensive and exotic ligands as well as the presence of transitionmetals as trace impurities in the final products, which restrictits practical applicability in the pharmaceutical industry. The development of novel, metal free pathways is presently an issue of significance in order to expand the frontiers of heterocyclic chemistryand has become the subjectof intense research among researchers. Therefore, to address the limitations of metal-catalysts and to design better synthetic pathways to construct C-C and C-N bonds for the synthesisand functionalization of important heterocyclic molecules we have developed metal-free strategies. The details of the work will be discussed in conference during lecture.



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IL-34

Current status leading to the discovery of drugs from medicinal plants

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The analysis into the sources of new drugs from 1981 to 2007 reveals that almost half of the drugs approved since 1994 were based on natural products. During the years 2005–2007, 13 natural product related drugs were approved. In the past decades, pharmaceutical industry focused mainly on libraries of synthetic compounds as drug discovery source as they are comparably easy to produce and resupply and demonstrate good compatibility with established high throughput screening platforms. However, high throughput screening (HTS) as the new drug discovery approaches did not fulfil the initial expectations and at the same time there has been a declining trend in the number of new drugs reaching the market. In 21st century the pharmacological effects of traditional medicinal plants have been considered as a promising source of future drug for the treatment of various challenging diseases and recently, there has been a resurgence of interest to rediscover medicinal plants as a source of potential drug candidate or lead molecule as the plants derived lead molecules have played an important role in pharmaceutical industries to optimize the activity of lead candidate in order to develop new effective drugs in treating the various diseases. Keeping in view importance of medicinal plants in therapeutic area and continuous of our ongoing programme to search the novel active plants constituents [1,2], recently we have isolated and identified the various lead molecules viz. novel anthraquinones, spirostane saponines, paederosides, bis-iridoid glucosides and triterpenoids from traditional medicinal plants. In this presentation current status leading to the discovery of drugs from medicinal plants, plant-derived drugs currently in markets and various active lead molecules and inactive plants constituents recently isolated and characterized in our laboratory will be discussed in detail.

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IL-35

Antibiotics from pond scum – exploring natural product biosynthesis in algae

Ellis O'Neill

Algae are well known to produce a wide range of high value compounds of benefit to human health, and can be grown relatively easily. Research is underway into the use of algae as nutritional supplements to enhance the diet of malnourished children and HIV-infected adults, for example. Algae also produce complex small molecules, which can act as toxins, anticancer agents and antibiotics. My research is on using novel analytical chemistry techniques to investigate the production and bioactivity of these more complex molecules by algae.

This work involves culturing a range of species and evaluating them for bioactivity, specifically looking for antibiotics. I also use high through put untargeted mass spectrometry and chemoinformatics to identify novel compounds produced by these species. The most promising compounds are then isolated and their structure solved.

With the increasing problem of antibiotic resistance, and with no novel antibiotics commercialised for decades, there is a growing imperative to discover new natural products. By focussing on these algae, which have not previously been investigated, I hope to be able to find previously undiscovered classes of compound that can be used as new medicines.

IL-36

Harvesting fused & functionalized azaheterocycles *via* metal-catalyzed and metal-free strategies: Promising pharmacophores for drug development

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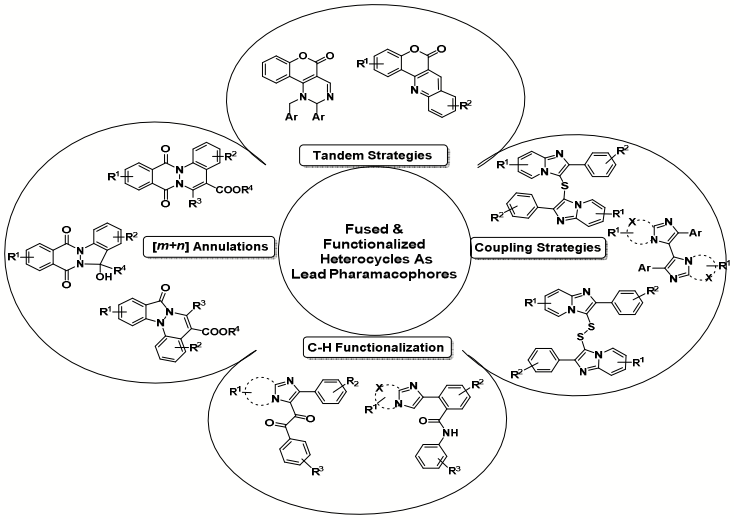
Fused and functionalized azaheterocycles are frequently found in numerous bioactive natural products, and have been intensively studied as drug candidates.[1] Accordingly enormous advancements have been made towards developing transition-metal-catalyzed and metal-free strategies for their synthesis as potential pharmacophores in the past few decades. However, limited molecules have proven their potential as active drug candidates owing to unpredictable outcomes in their preclinical/clinical research phase studies of drug development process. Despite great efforts, the development of direct synthetic strategies facilitating the building of useful molecular architectures in minimum steps *via* modern flourishing organic chemistry is highly desirable and challenging.
Our continuous efforts[2] in this direction have led to the discovery of interesting azaheterocycles with unprecedented structures prepared at the expense of (a) cross-coupling reactions, (b) direct functionalization, (c) cross-dehydrogenative coupling, and (d) annulation *via* C-H activation protocols in a tandem manner, which shall be discussed.



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IL-37

Dibridgehead Diphosphine Cage as Molecular Receptor for Precious Metal Capture and Transport

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The dibridgehead diphosphine $P((CH_2)_{14})_3P$ (**1**) have ability to turn itself inside-out to give a mixture of *in*,*in* and *out*,*out* isomers.[1] This isomerization is referred as homeomorphic isomerization.[2] Since the lone pairs are directed in an *exo* sense in *out*,*out*-**1**, and an *endo* sense in *in*,*in*-**1**, we thought that such diphosphines might be used in scavenging suitable Lewis acids and possibly transport them as payloads to an orthogonal phase.[3] To confirm this hypothesis a U-tube experiment is designed. In these experiments, U-tubes are charged with CH_2Cl_2 solutions of **1** (lower phase), an aqueous solution of K_2MCl_2 (charging arm; M = Pt, Pd), and an aqueous solution of excess KCl (receiving arm). The MCl_2 units are then transported to the receiving arm until equilibrium is reached. When the receiving arm is charged with KCN, transport is much faster and higher K_2MX_2 equilibrium ratios are obtained ($\geq 96 \leq 4$). Analogous experiments with K_2PtCl_2/K_2PdCl_2 mixtures in charging arms show $PdCl_2$ transport to be faster. No transport occurs in the absence of **1**, and other diphosphines or mono phosphines assayed give only trace levels.

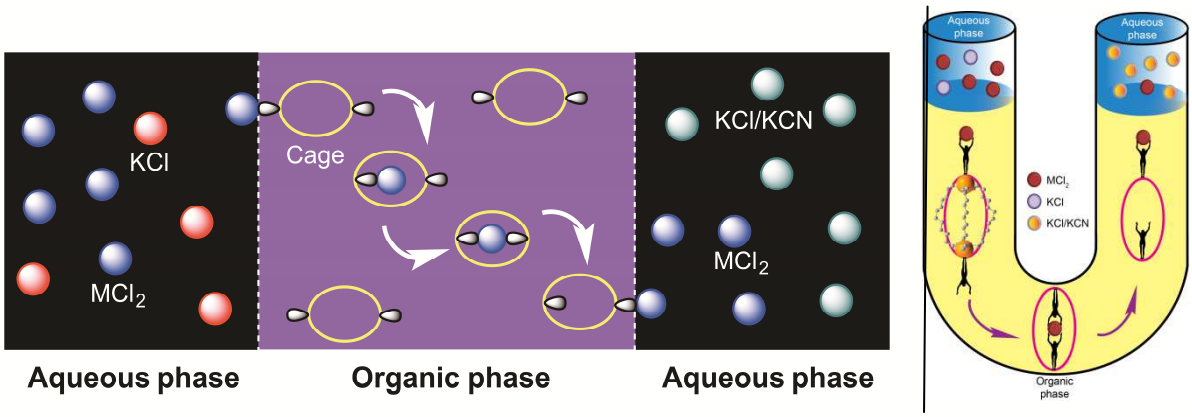

Figure 1. Schematic Representation of Precious Metal Capture and Transport by Dibridgehead Diphosphine Cage.

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IL-38

Synthesis of various arylated benzenes from 2-(1-arylethylidene)-malononitriles

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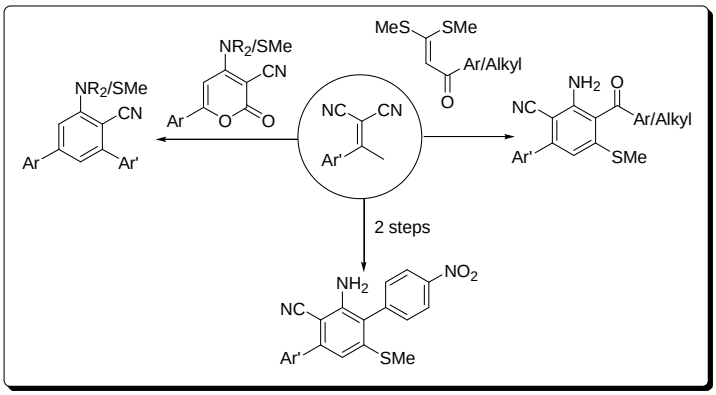
ABSTRACT:



α,α-Dicyanoolefins are readily accessible compound through Knoevenagel reaction of the corresponding aromatic/heteroaromatic/aliphatic ketones with malononitrile.[1] These compounds are widely used in synthetic organic chemistry due to their use as Michael acceptors[2] as well as source of nucleophile.[3] Various reactions of 2-(1-arylethylidene)malononitriles were reported for the establishment of the multifunctional moieties.[4-10] These compounds were subjected to various chemical reactions, such as reaction with α,α-dicyanoolefins to afford benzene,[4] allylic alkylation with Morita–Baylis–Hillman carbonates,[5] direct asymmetric vinylogous for Mannich reaction,[6] allylic amination,[7] [3+2] annulation,[8] γ-trifluoromethylation[9] and asymmetric Michael addition reaction.[10] Herein, we have used α,α-Dicyanoolefins as a precursors to develop differently functionalized arylated benzenes. We have successfully synthesized biaryls and p-teraryls.

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IL-39

Fluorine Chemistry–An important tool for new drug discovery program in the 21st century

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IL-40

Science and Technology trends in Biologics

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In past one decade, the research in Biologics has rapidly grown and unlocked new directions for the diagnosis and treatment of diseases, due to robust pharmacological activities, low toxicity, minimal side effects and high target specificity.

Study shows that persistent innovation and rapid progress in the areas of biologics- related biotechnology, have heightened awareness of its market prospects and potential for transformation of the Healthcare and Medical fields.

Medical biotherapy, involving the use of biologics for treatment of various diseases including cancer, auto-immune diseases, inflammation, infectious diseases, endocrine diseases and cardiovascular diseases has become and important emerging field. Biotherapy has become the important emerging field.

Despite their potential benefits, biologics present challenges due to their fragile biology and demand for complex manufacturing conditions and processes.

Top five countries for publishing research papers in Biologics are United States, China, Japan, Britain, and Germany, while India Ranks 13th in the list.

This paper will discuss trends in Biological research is in the fields of therapeutic antibodies, fusion proteins, gene therapy, cell therapy and vaccines.

Data is based on scientific papers and patents provided by Chemical Abstracts Service (CAS) – a div of the American Chemical Society, USA.

IL-41

Bacteria Fighting Back: Structural Basis for Function of the Staphylococcal Peroxidase Inhibitor

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Abstract: *Staphylococcus aureus*secretes an array of proteins, many of which serve to disrupt the host's innate immune system from recognizing and clearing bacteria with optimal efficiency. Our collaborator Dr. Geisbrecht's laboratory has identified a novel immune evasion protein and named it SPIN, for Staphylococcal Peroxidase Inhibitor.SPIN is a previously uncharacterized protein which is found only in Staphylococci. This protein binds tightly to human enzyme myeloperoxidase (MPO) and contributes bacterial survival following phagocytosis. The heme-containing enzyme MPO is critical for optimal antibacterial activity of human neutrophils. The major role of SPIN is toprevent MPO-driven production of toxic hypohalous acids that are directly bactericidal. Our recent studies have provided insights into SPIN structure/function relationship and deepen our understanding of bacterial escape from the innate immunity. These studies also constitute a template for the design of synthetic MPO inhibitors which could prove useful for anti-inflammatory applications.

IL-42

Open flask, catalyst-free synthesis ofoxindole containing α-hydroxy phosphinoyl compounds

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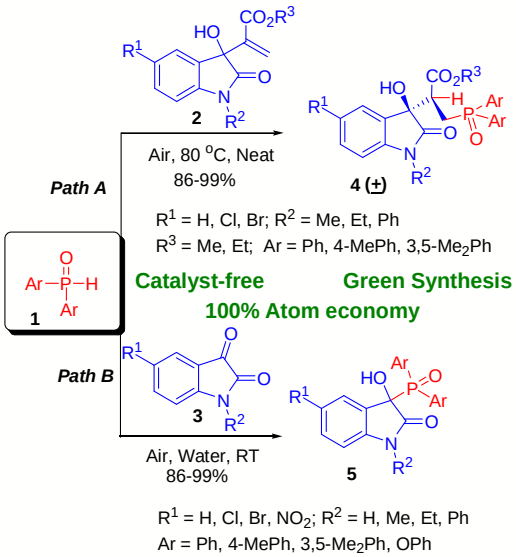
Abstract: Due to their versetaile applications in the organic synthesis, organometallic chemistry, medicinal chemistry, chemical biology, and material science, cleaner and more efficient methods for the syntheis of organophosphorus compounds need to be developed.[1] An open flask, air induced diastereoselective C-P bond formation between phosphorous surrogates **1** and oxindole containing allyl alcohols (**2**) under catalyst-free and solvent-free conditions is described (Path A).[2] The protocol was further extended to the C-P bond formation between phosphorous surrogates **1** and isatin derivatives **3** (Path B).[3] The resulting products **4**&**5**were obtained in excellent yields.



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IL-43

Enantioselective Unified Oxidative Cyclization strategy to Diverse Carbocyclic scaffolds

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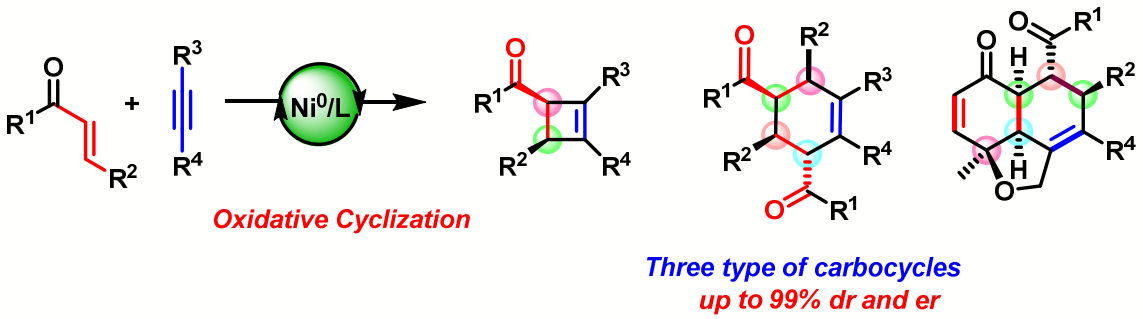
Given the importance of chiral carbocyclic molecular structures in medicinally importantnatural products, development of step-economical and unified synthetic strategy is an important area of fundamental research. Oxidative cyclization of unsaturated components, such as alkenes, alkynes etc. on nickel provides a unique tool to access carbo- and hetero-cycles of diverse pattern, depends upon coupling partners. In this presentation, development of catalytic and enantioselective methods will be demonstrated, which provides an efficient and unified strategy to access chiral cyclohexenes and cyclobutenes with two and four chiral centers, respectively in highly diastereo- and enantioselective manner.[1]A desymmetrization strategy will also be demonstrated to access chiral tricyclic fused rings with five contiguous chiral centers.[2]Step-economical, complete control of selectivity and cheaply available feedstock starting materials are the salient features of the above developed method.



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IL-44

Versatility of carbon disulfide: Greener synthetic strategies for biologically potent scaffolds

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Abstract: Structurally diverse organosulfur compounds displayed plethora of important applications such as pharmaceuticals, agrochemicals, intermediates in organic synthesis and also has been employed as a useful synthons for the generation of structurally diverse biologically potent scaffolds.[1] Many of them have been approved as drugs, prodrugs and drug candidates. Keeping the view of importance of these compounds, extensive efforts have been made by the scientists around the globe to generate various kinds of structurally diverse organosulfur compounds from simple to the complex molecules employing traditional methodologies such as use of thiophosgene and its derivatives, which are harmful reagents. In recent years, carbon disulfide has been emerged as a cheap and safe alternative to generate various kinds of structurally diverse biologically potent organosulfur scaffolds employing various kinds of reagents and catalytic systems. In the present talk,[2] I would like to discuss some of our recently reported novel and efficient synthetic methodologies for the synthesis of acyclic biologically potent organosulfur scaffolds such as dithiocarbamates, trithiocarbonates, dithiocarbazates etc., employing carbon disulfide and a variety of reagents and catalytic systems.

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ORAL

O-1

Quantification of Hydrogen Bond Strength Based on Interaction Coordinates: A New Approach

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Choice of Presentation Mode: Oral (Podium) Presentation
Name and date of birth of the presenting author: Dr. Sarvesh Kumar Pandey (09/01/1988)

Abstract: The existence of life depends on bulk water and biomolecular aggregates. It is well known that the noncovalent interactions play a vital role in deciding the structure and properties of chemical and biological systems.[1] One of the important noncovalent interactions having a profound effect is the hydrogen bond (HB). Encouraged by our recently reported proposal,[2] a new approach to quantify hydrogen bond strengths based on interaction coordinates (HBSBIC) is proposed and is very promising. In this research, it is assumed that the projected force field of the fictitious three atoms fragment (D—H···A) where D is the proton donor and A is the proton acceptor from the full molecular force field of the H-bonded complex characterizes the HB. The "interaction coordinate (IC)"[3] derived from the internal compliance matrix elements of this three-atoms fragment measures how the D—H covalent bond (its electron density) responds to constrained optimization when the H···A hydrogen bond is stretched by a known amount(its electron density is perturbed by a specified amount). This response of the D—H bond, based on how the IC depends on the electron density along the H···A bond, is a measure of the hydrogen bondstrength (HBS). The inter- and intramolecular HBSs for a variety of chemical and biological systems are reported.[4] When defined and evaluated using the IC approach, the HBSBIC index leads to satisfactory results. Because this involves only a three-atom fragment for each HB, the approach should open up new directions in the study of "appropriate small fragments" in large biomolecules.

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O-2

Synergistic Role of Carbonaceous Reinforcements on Multi-Length Scale Tribology of Electrophoretically Deposited Nickel-Boron Nitride Coatings

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Abstract: Nickel with chemically and thermally stable hexagonal boron nitride (Ni-BN) is used as dry lubricant coating for high technology applications of automotive and aeroengines [1, 2]. Multi length scale tribological studies can be inalienable for the wide range of applications at different scales; from macro to micro scales technologies, for example, tribology of multi layered structures and materials, micro machining, laser texturing etc. [3]. Catastrophic failure of the materials can caused due to the enhanced vibrations in fretting wear (macro scale tribology). Thus, the estimation of fretting wear is indispensable to maintain the service life of materials, involved in engineering applications [4]. However, the micro-scratch testing (micro scale tribology) can be used as alternative tool for the quantitative assessment of the adhesion strength of the coatings, waning in which restricting applicability and life time of the coating. Therefore, the emphasis of the current work is to investigate mechanical and multi length scale tribological aspects of electrophoretically deposited nickel with synergistic reinforcement of hexagonal BN along with different carbonaceous additives like graphene (Ni-BN-Gr), carbon nanotubes (Ni-BN-CNT) and diamond (Ni-BN-D). Highest hardness and elastic modulus of Ni-BN-D coating than that of Ni-BN-CNT, Ni-BN-Gr and Ni-BN coatings was linked to their high compressive stress, dislocation density and yield strength (calculated by Taylor's model). Addition of graphene, CNT and diamond in Ni-BN composite divulged a decrease in wear volume due to the synergetic lubricating effect of BN and carbonaceous reinforcements. The friction mechanism for the coatings during micro-scratching was predicted by friction model and the contribution of ploughing and adhesion components was compared with the experimental frictional values. Thus Ni-BN-D restrict inception of wear at different length scale and can be a potential three phase metal-ceramic coating for engineering and industrial applications.

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O-3

Biochemical Characterization of Fc-Fusion Protein Conformers

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Abstract: Bispecific antibodies and fusion proteins are novel biologics that combine the specificities of two different molecules and simultaneously target two epitopes. Such biologics with 'two target' functionality can interfere with multiple surface receptors and aid in enhanced bio-therapeutic efficacy. Assembling a bispecific molecule from two different parental molecules expressed in the same producer cell may result in various non-functional forms with respect to bispecificity.
Here we look into the active and inactive forms of a bispecific Fc-fusion protein. A mass spectrometric analysis of IdeS subunitsrevealed the identical amino acid sequence of the two forms, butsignificant differences in inter-chain hinge region disulfide bonding and some variations in *O*-linked glycosylation. Majority of the inactive form was found to lack inter-chain hinge region disulfide bonds and therefore present as 'half-molecules'.SE-HPLC analysis was performed on 40^{o}C heating time-course samples, where a rapid formation of 'half-molecules' for the inactive form validates the previous findings. Interestingly,the hinge region cysteines were all in oxidized form as shown by peptide map LC-MS analysis, indicating the occurrence of intrachain disulfide bond shuffling, instead of simple under-disulfide bonding.Disulfide bond mapping is currently underway to resolve the detailed disulfide bonding structures of both active and inactive forms. Intrinsic tryptophan fluorescence studyhas shown the upper level structural differences between the two,and further biophysical characterization will be performed to demonstrate the inactive form is a conformer of the active form.

O-4

Electrospun woven antibacterial wound healing mats synthesized with norfloxacin imprinted polymer nanofibers

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Abstract: Wound healing treatment of topical skin ulcers remains a global healthcare issue.The various current strategies are employed to treat to the ~ 8 million patients of chronic wounds. Furthermore, the bacterial infection may enhance the severity of wounds. Thus, norfloxacin, a synthetic chemotherapeutic antibacterial agent of the fluoroquinolone family, is employed as a skin replacement material to be used in wound healing and/or burn dressing. This study explores the fabrication of electrospun woven wound healing mats with norfloxacin imprinted nanofibers towards accelerating the wound healing process. Notably, the molecularly imprinted polymer nanofibers (MIP-NFs)have beenextensively studied owing to their unique features including sustained drug release, high drug loading capacity, increased mass transfer rate, flexibility in surface properties, biocompatibility, and high mechanical strength. The electrospun norfloxacin imprinted polymers with a biocompatible backbone polymer (i.e., matrix polymer) will be fabricated and characterized via a series of analytical techniques. The fine tuning of imprinting methods, electrospinning process, and hydrophilicity of MIP-NF mats may govern the interactions occurring at material-biology interface, eventually resulting into higher amount of sustained norfloxacin release as compared to non-imprinted nanofibers (NIP-NFs) mats and matrix polymer only nanofibers. Finally, the norfloxacin *in vitro* release and antibacterial activity of these MIP-NFs will beevaluated against *Escherichia coli*toevaluate their biomedical utility in wound healing processes.

O-5

Copper (II) dimers stabilized by bis(phenol) amine ligands: Theoretical and Experimental Insights

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Abstract: Using deprotonated forms of tetradentatebis(phenol) amine ligands 2–(((3,5–di–tert–butyl–2–hydroxybenzyl)(2–hydroxyethyl)amino)methyl)–4,6–di–tert–butylphenol ($^{2}LH_2$) and newly synthesized Methyl–2–(bis(3,5–di–tert–butyl–2–hydroxybenzyl)amino) propanoate ($^{1}LH_2$),dinuclear copper(II) complexes were synthesized. These ligands yielded two binuclear complexes of composition [($^{n}L)_2Cu^{II}_2$][{n = 1, (**1**) and n = 2, (**2**)] which have been characterized by X–ray crystallography, UV–Vis and magnetic susceptibility measurements. The phenolate moieties of the copper complexes were electrochemically oxidized to phenoxyl radicals. The antiferromagnetic exchange coupling of two copper centers of these complexes has been investigated by magnetic susceptibility (2–300 K) measurements. The weak exchange coupling constants (*J*) of these complexes, when compared to the literature values, is most likely attributed to the smaller Cu···Cu distance and Cu–O(Ph)–Cu angle. [$^{1}LCu^{II}$(py)] (**4**) and [$^{2}LCu^{II}$(py)] (**5**) show rhombic spectra typical of d^9 configuration. The dimer complex can be converted into the corresponding monomeric Cu(II) complex, [$^{1}L_2Cu^{II}_2$(X)] (X = py), by adding an exogenous ligand such as pyridine (py) into a CH_2Cl_2 solution of the dimer. All EPR spectra have been simulated and analyzed. The cyclic voltammograms observed with $^{1}L_2Cu_2$ and $^{2}L_2Cu_2$ revealed two oxidations with a similar small difference in their redox potentials.Since a copper(II)–oxidation is not feasible at such low potentials, these redox processes were assigned to ligand–centered oxidation yielding phenoxyl radical in the complex. Density Functional Theory (DFT) at the B3LYP level and Time-Dependent (TD)-DFT calculations rationalize the electronic structure of the complexes and throw light on the origin of observed electronic transitions.

O-6

Six-coordinate $[Co^{III}(L)_2]^z$ complexes (L(2–) = azo-appended*o*-aminophenolate; z = 1–, 0, 1+): molecular and electronic structure

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Abstract: The interplay of transition-metal ions and proradical ligands in general and *o*-aminophenolate-based ligands in particular, and the correlation of reactivity with electronic structure, is an area of significant current research interest.[1] Formation of the tyrosyl radical in mononuclear copper enzyme galactose oxidase is a prototypical example of a class of metalloproteins to use free radicals as cofactors to promote oxidation reactions.[2] Redox-active ligands offer an intriguing way to approach multielectron reactivity at a well-defined metal complex and play a role in catalysis.[3] *o*-Aminophenolate-based ligands span redox-levels from dianionic *o*-amidophenolate $(L^{AP})^{2-}$ to *o*-iminosemiquinonate(1−) monoanion $(L^{ISQ})^{\bullet-}$ π- radical to neutral *o*-iminoquinone $(L^{IBQ})^0$ forms. Over the years, the number of coordination complexes of *o*-aminophenol-based ligands has expanded enormously from initial bidentate to tri-, tetra-, penta-and hexa-dentate.[4-6] In this work we directed our attention to exploring the coordination ability of new redox-active ligand towards cobalt. We report here on the synthesis, structural characterization, cyclic voltammetry and spectral (^{1}H NMR, ESI-MS, EPR and UV-VIS-NIR) properties of three new complexes $[Co(L^1)_2]$ **(1)**, $[Co(L^1)_2][PF_6]\cdot 2CH_2Cl_2$ (**2**) and $[Co^{III}(\ ^5\text{-}C_5H_5)_2][Co(L^1)_2]\cdot MeCN$ (**3**).

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O-7

Survival and proliferation improves of liver sinusoidal endothelial cells transplanted in mice by endothelin receptor antagonism

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Abstract: Liver sinusoidal endothelial cells are critical for homeostasis, repair and regeneration of liver. These contribute coagulation factors, paracrine signals and other functions that may be reconstituted by cell transplantation approaches. As oxidative and inflammatory mechanisms rapidly diminish endothelial cell survival, it is important to determine whether this could be modulated. In endothelial injuries multiple evidences incriminate endothelin receptors; thereby suggesting cytoprotection could be prospectively achieved by existing ETA/B antagonists. We used mouse liver sinusoidal endothelial cells in transplantation and other assays to investigate this possibility with ETA/B blocker, bosentan. Dipeptidyl peptidase IV deficient (DPPIV-) knockout mice received hepatic preconditioning for promoting cell engraftment and proliferation. We analyzed cell viability, mitochondrial function, injury responses and cell proliferation. After ETA/B antagonism, endothelial cells maintained better viability. ETA/B antagonism improved mitochondrial membrane potential, increased ability to withstand oxidative stress and lessened DNA damage susceptibility. Endothelial cells with ETA/B antagonism followed by transplantation in liver showed significantly greater engraftment. In endothelial cells transplanted under liver repopulation conditions, ETA/B antagonism accelerated the proliferation kinetics. Importantly, ETA/B antagonism increased expression of ataxia telangiectasia mutated protein with coordination of downstream signaling. This regulates mitochondrial homeostasis and protects from DNA damage. ETA/B antagonism with bosentan protected liver sinusoidal endothelial cells. In this cytoprotection, ataxia telangiectasia mutated pathway imparted superior mitochondrial function, DNA integrity and resistance to injuries. ETA/B antagonism will advance development of cell interaction models, mechanisms in liver regeneration, and cell therapy applications. Extensive clinical experience with ETA/B antagonists will facilitate translation in people.

O-8

Ascorbate peroxidase and its role in the transformation of methyl phenyl sulfide to its sulfoxide.

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Abstract: Synthesis of chiral sulfoxide is an active area of continuing research interest. The most common method for the preparation of sulfoxides is by the oxidation of their corresponding sulfides. Both the chemical and biological catalysts have been developed for this purpose. Though the reaction conditions for the preparation of chiral organic sulfoxides involving biological catalysts are milder and ecofriendly in comparison to those involving chemical catalysts, they are of limited practical use. The whole cell cultures of bacteria, fungi and yeast as well as isolated enzymes have been used to oxidize organic sulfides to their corresponding sulfoxides in good enantiomeric excess in specific cases. Studies suggest that specific biological catalysts could oxidize specific organic sulfides to their sulfoxides in good enantiomeric excesses

An ascorbate peroxidase from a new source *Musa paradisiaca* leaf juice has been purified to homogeneity using a simple procedure involving concentration by ultra filtration and anion exchange chromatography on diethyl amino ethyl [DEAE] cellulose column. Sodium dodecyl sulphate-polyacrylamide gel electrophoresis [SDS-PAGE] analysis of the purified enzyme has shown a single protein band of molecular mass 208.9kDa which has been confirmed by native-PAGE and intact mass analysis by mass spectrometry. The enzymatic characteristics like Km for the substrates sulfide and H_2O_2, pH and temperature optima of the enzyme have been determined. The enzyme transformed approximately 97% methyl phenyl sulfide to its sulfoxide. The results of the above studies will be presented in the conference
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Key words: Plant peroxidase, Musa paradisiaca, methyl phenyl sulphide, Metalloenzyme.

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O-9

Baylis–Hillman Acetates in Synthesis: Copper(I)/tert-Butyl Hydroperoxide Promoted One-Pot Oxidative Intramolecular Cyclization Protocol for the Preparation of Pyrrole-Fused Compounds and the Formal Synthesis of (±)-Crispine A

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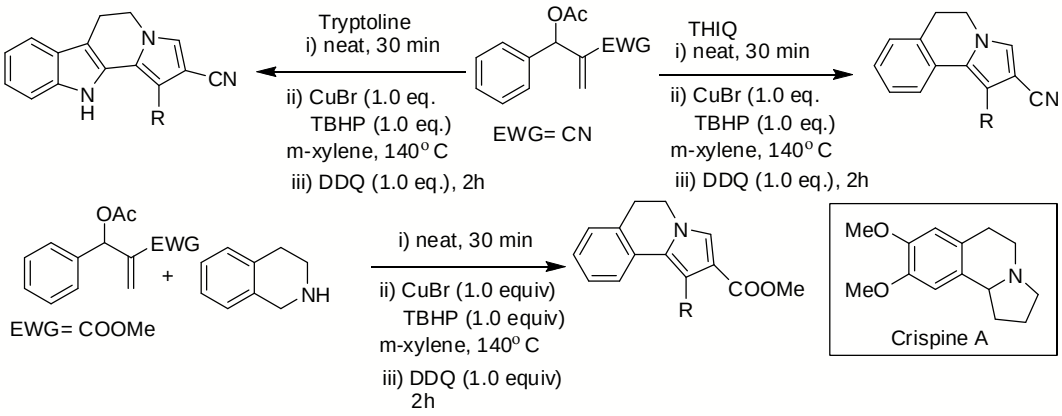
Abstract: The benzo-fused indolizine(pyrrolo[2,1-a]isoquinoline) and indole-fused indolizine(indolo[2,3-a]indolizine) frameworks are present in various natural products and several biologically active molecules. In continuation of our interest on the BaylisHillman reaction,[1-4]we have presented here a facile onepot CuI/tert-butyl hydroperoxide (TBHP) promoted intramolecular 1,5-electrocyclization and oxidative aromatization of in situ generated allylamines from Baylis–Hillman acetates for the synthesis of both pyrrolo[2,1-a]isoquinolines and indolo[2,3-a]indolizines. This methodology was further extended by the formal synthesis of (±)-crispine A.[5] This study demonstrates the application of Baylis–Hillman acetates in organic and medicinal chemistry.



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O-10

Green approach for the synthesis of 1, 4-dihydropyridine moiety and their biological assay

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Abstract: A one-pot multi-component procedures for the preparation of highly functionalized 1,4-dihydropyridines from different heterocyclic aldehydes, ammonium acetate and different β-ketoesters under catalyst-free and/or solvent-free conditions were described. All the synthesized products were confirmed by ^{1}H-NMR, ^{13}C-APT and IR spectroscopy studies. A brief single crystal study of selected compounds was reported. The produced scaffolds were screened for their biological assay and some of the compounds show significant outcomes.

O-11

Designing of Smart Fluorescent Probes for Bio-imaging and Diagnostics

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Abstract: Recently, there has been a lot of interest in the development of fluorescent probes for bio-imaging and identification of diseases. In our body, diseases arise due to abnormal changes in gaso-transmitters (H_2S and NO) and intracellular viscosity. Thus, designing of fluorescent probes which can monitor gaso-transmitters and intracellular viscosity may acts as a tool for diagnosis of many diseases. In this context, we have designed a fluorescence probe for monitoring of H_2S induced apoptosis.[1] Here, utilizing this probe, we for the first time reported a dual functional strategy for the detection of endogenous H_2S and its anticancer effect in living cells. For monitoring of nitric oxide (NO), we designed lysosome targetable probe which detects NO in living cells as well in rat brain tissue.[2] We then utilized this probe for monitoring of enzymatically generated NO levels at variable tissue depths. For the detection of neurotoxic aluminum ions, we reported a solid state luminescent probe which detect aluminum ions in solution as well as in solid state and is further utilized for *in vitro* and *in vivo* applications.[3] Further, for the diagnosis of diseases like cancer and apoptosis, we reported a smart strategy based on molecular rotation of *meso*-substituted bodipy.[4] Using this molecular rotor, we explored an easy and economical approach for identifying diseased cells out of normal cells on the basis of changes in intracellular viscosity

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3. 3 **N. Gupta**, T. K Kaur, V. Bhalla, R. D. Parihar, P. Ohri, G. Kaur and M. Kumar. *Chem. Commun.*, 2017, **53**, 12646.
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O-12

Rhodium catalyzed stereospecific reductivecarbocyclization of 1,6-enynes for the synthesis of entecavir-aristromycin hybrid analogs

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Abstract: Hepatitis B virus (HBV) infection is still not curable and need for long-term treatmentwhichmandates identification ofnovel and selective inhibitors of HBV replication.The 6'-exo double bond is an essential pharmacophore for anti-HBV activity of Entecavir, a most potent marketed drug to treat HBV inflection. Aristeromycin, a naturally occurring carbocyclic nucleoside haswide range of antiviral activities. Owing to the importance of aristeromycins and entecavir as antivirals, we combined their features including 4' substitution to generate newentecavir-aristromycin hybrid analogs.BINAP directed rhodium catalyzed reductive carbocyclization of 1,6-enynes through asymmetric hydrogenation was explored for the construction of the target entecavir-aristromycin hybrid analogs.

Recently, there has been a lot of interest in the development of fluorescent probes for bio-imaging and identification of diseases. In our body, diseases arise due to abnormal changes in gaso-transmitters (H_2S and NO) and intracellular viscosity. Thus, designing of fluorescent probes which can monitor gaso-transmitters and intracellular viscosity may acts as a tool for diagnosis of many diseases. In this context, we have designed a fluorescence probe for monitoring of H_2S induced apoptosis.[1] Here, utilizing this probe, we for the first time reported a dual functional strategy for the detection of endogenous H_2S and its anticancer effect in living cells. For monitoring of nitric oxide (NO), we designed lysosome targetable probe which detects NO in living cells as well in rat brain tissue.[2] We then utilized this probe for monitoring of enzymatically generated NO levels at variable tissue depths. For the detection of neurotoxic aluminum ions, we reported a solid state luminescent probe which detect aluminum ions in solution as well as in solid state and is further utilized for *in vitro* and *in vivo* applications.[3] Further, for the diagnosis of diseases like cancer and apoptosis, we reported a smart strategy based on molecular rotation of *meso*-substituted bodipy.[4] Using this molecular rotor, we explored an easy and economical approach for identifying diseased cells out of normal cells on the basis of changes in intracellular viscosity.

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O-13

Startup Opportunities in Chemistry-Biology Interface

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Abstract: Start-up opportunities in the interface of chemistry and biology have been steadily rising. With growing start-up ecosystem in India, govt has made significant headway in creating ample opportunities for the scientists to take their research to market. The number of start-ups in India has grown rapidly over the last few years and making impact by improving people's health through science and innovation. As scientist working in the interface of chemistry and biology it is important to direct our research and innovation to impact the society and aid in solving the problems of our society. Academia will continue to be central source of life science research and innovation, we must find new ways to encourage ourselves to explore research ideas and take the risks necessary to make it translational i.e make it available to society. We should take interdisciplinary and innovative approach to integrate our research for the betterment of our lives. This talk would be focusing on several initiatives taken up by government (BIRAC schemes and schemes from DST) and entrepreneurship opportunities available in Indian for all scientists to collaborate among ourselves and start a new venture that can create impact.

O-14

Chemoselective Iodination of Alkynes using Sulfonium Iodate (I) Complex

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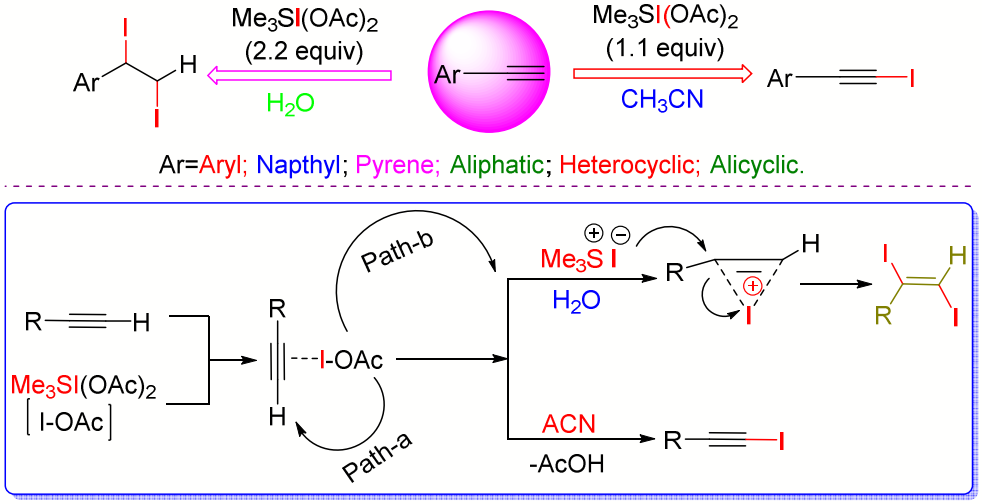
Abstract: Iodo-functioctionalized molecules have gained considerable attention due to their synthetic usefulness as key intermediates and valuable synthons in organic chemistry.[1]In particular, 1-iodoalkynes represent important subclass which have been widelyinvolved as useful precursors in several attractive chemical transformations,[2] Nozaki-Takai cross coupling,[3]Hetero-functionalization *via* CuAAC"Click reaction", total syntheses of active natural products and biologically active molecules.[4,5]Iodoalkyne derivatives also served as promising chemical probes of outmost pharmaceutical applications such as *anti*-HIV, *anti*-microbial, and fungicidal agents.[6]
During our research,[7] we developed a novel and efficient method of iodination of alkyne using Sulfonium Iodate (I) electrophilic reagent under metal-free conditions. This stereo-divergent approach is amenable to a wide range of alkyne substrates and demonstrates a diverse functional group tolerance resulting in synthetically valuable 1-iodoalkyne and *(E)*- vicinal-diiodo alkenesin good to excellent yields (up to 99%) with 100% selectivity under ambient conditions.[7d]



Selective iodo-functionalization using the sulfonium iodate(I) reagent system

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O-15

‘‘Sulfonium Iodate Reagent MediatedStereoselectiveSynthesis of 2-Deoxy Glycosidesand Glycoconjugates’

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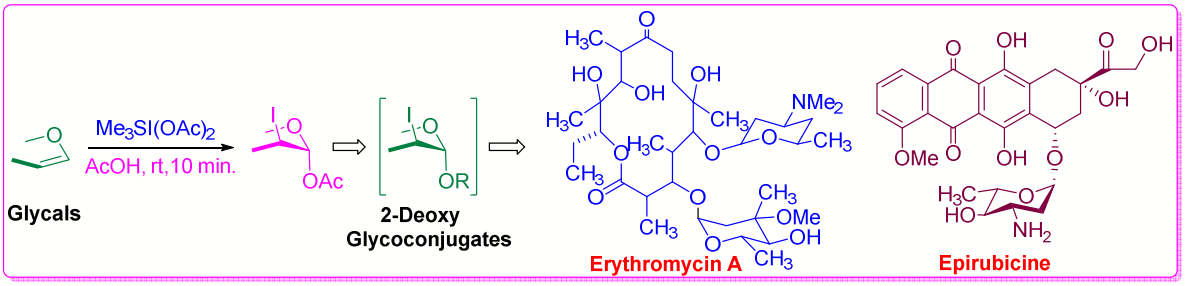
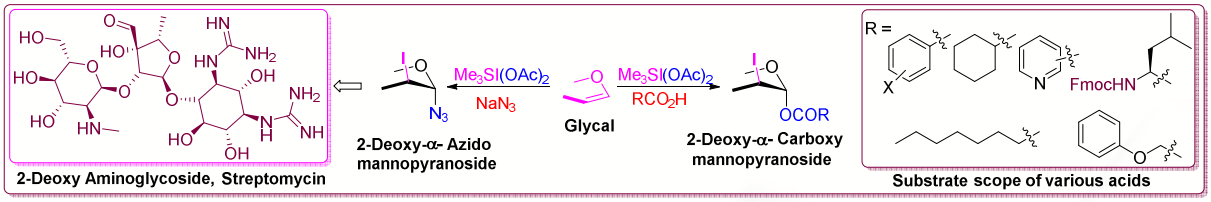
Abstract: 2-Deoxy sugars and their derivatives have been recognized as important synthetic intermediates for constructing several valuable glycoconjugatesand natural products.The presence of or linkage in 2-deoxy glycosides plays a crucial role in molecular recognition, reactivity, and adhesion of glycosubstances and linked to several cellular processes. In this context, stereoselective glycosylation strategies serve as an important chemical tool for assembling venerable sugar molecules and related natural products to probe their biological activities.

Herein, we repoteda simple, efficient, method developed for the synthesis of 2-deoxy-2-iodo glycosides and glycoconjugates using sulfonium-salt reagent system. $Me_3SI(OAc)_2$ is effectively prepared from Me_3SI and $PhI(OAc)_2$, to access the one-potiodoacetoxylation,iodocarboxylation using carboxylic acids, and iodoazidation using NaN_3 or $TMSN_3$.The extension of the reagent was examined for a broad range of substrates, including various substituted aromatic carboxylic acids, heterocyclic, alicyclic, and aliphatic carboxylic acids, and amino acids to obtain various glycoconjugates in high yields (99%) with diastereoselective ratio up to 100%.





$Me_3SI(OAc)_2$ promoted one-pot Iodocarboxylation and Iodoazidation:

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O-16

Novel, facile and green approach towards synthesis of Imidazolocoumarin derivative

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Abstract: Herein we report an aqua mediated cyclization protocol against the reported process of hitherto hybrid scaffolds ofcoumarin and imidazole core. The synthetic methodology initiates with linking of aromatic amines with 3-nitrocoumarin at 4-position, followed by reductive cyclization using sodium dithionite leading to the formation of title compounds in high to excellent yields (70-80%). Detailed characterization including ^{1}H NMR, ^{13}C NMR and for all newly synthesized reference compound has been reported.

O-17

Diphenylethylenediamine-Based Potent Anionophores: Transmembrane Chloride Ion Transport and Apoptosis Inducing Activities

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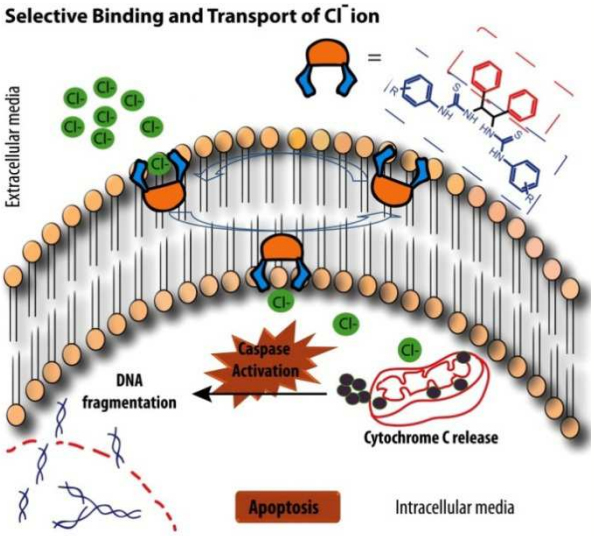
Abstract: Synthetic anionophore research has drawn the attention of many chemist, biochemist and as well as supramolecular chemist as this area of research has a huge impact on therapeutic application.Ion transportation across the cell membrane plays a pivotal role in regulating the various physiological function like cell signaling pathways, proliferation, ion-homeostasis, cytosolic pH and other cellular processes.[1]The Chloride channel is one of the most important pore-forming membrane protein that allows the passive transport of Cl^-ion across biological membranes. It is essential for the regulation of cell volume,transepithelial transport of salt and water, modulation of the electrical excitability in neurons.Even a small aberration in chloride channel can overwhelm these cellular processes and may cause lot of deadly disease like myotonia , best disease, startle disease, barter's syndrome, epilepsy, cancer and others. Reduction of epithelial chloride conduction through various CFTR-channel leads to one of the most life threatening disease called cystic fibrosis.[2]Recent studies showed thatby disrupting cellular ion homeostasis, the synthetic Cl^-ion transporters can induce apoptosis in cancer cell lines, leading to a revived attention for synthetic Cl^-ion transporters.[3]



Herein, we report the development of conformationally controlled 1,2-diphenylethylenediamine-based bis(thiourea) derivatives as a new class of selective Cl− ion carrier. The strong Cl− ion binding properties (K_d= 3.87−6.66 mM) of the bis(thiourea) derivatives of diamine-based compounds correlate well with their transmembrane anion transport activities (EC50 = 2.09−4.15 nM). The transport of Cl− ions via Cl^-/NO_3^- antiport mechanism was confirmed for the most active molecule. Perturbation of Cl− ion homeostasis by this anion carrier induces cell death by promoting the caspase-mediated intrinsic pathway of apoptosis.

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O-18

Synergism between Novel Immunomodulators and Chemotherapy for the Cure of Experimental Visceral Leishmaniasis

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Abstract: Miltefosine is the mainstay of the visceral leishmaniasis (VL) elimination program in the Indian subcontinent but its narrow therapeutic index and long half-life may promote the resistance development and constrain its extensive use [1-2]. Moreover, rejuvenation of deteriorated host immune functions is crucial for successful eradication of *Leishmania* parasites [3]. Thus, the use of immunomodulator(s) in combination with Miltefosine may facilitate the restoration of host immunity and overcome the monotherapy-associated adverse effects [4]. In this milieu, we investigated the therapeutic and immunomodulatory potential of Leptin (50 µg/kg for 5 days, intraperitoneal dose) and Lentinan (2.5 mg/kg for 5 days, intraperitoneal) either alone or in conjunction with 8-times lower dose of miltefosine (2.5 mg/kg for 5 days, oral) on *Leishmania donovani* infected Balb/c mice. The hepatic and splenic parasite burden was evaluated by Giemsa staining method. Th1/Th2 cytokines, IgG responses, NO and ROS level, phagocytic activity and T-cell proliferation were determined by ELISA, Griess assay, flow-cytometry and XTT assay, respectively on day 7 post-treatment. Our results demonstrated that animals which received Leptin+Miltefosine or Lentinan+Miltefosine therapy showed almost 100% inhibition of *Leishmania* parasites. Both combination groups displayed significantly increased level of Th1 cytokines (IFN-γ, IL-12 and TNF-α) along with nitric oxide and notably suppressed level of Th2 cytokines (IL-10, IL-4 and TGF-β). Furthermore, maximum IgG2 antibody level, splenocyte proliferation and induced phagocytic ability of macrophages were evidenced during combination therapy when compared with other treated groups. In conclusion, these adjunct therapies could be promising alternatives for VL treatment, with an establishment of strong cell-mediated immunity

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O-19

EXPLORATION OF A NOVEL CHEMICAL CROSS-LINKER FOR THE TREATMENT OF KERATOCONUS

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Introduction

Keratoconus is a corneal ectatic disorder wherein the cornea becomes weak and cone shaped leading to defective vision in the form of severe astigmatism. This study developed a chemical cross-linker containing EDCI, NHS and Suberic acid to cause corneal cross-linking without removing the corneal epithelium or the use of UV-A irradiation, in turn avoiding the risks associated with the conventional treatment for keratoconus.

Methods

We analyzed the cell death and the phenotype of cells in the corneal layers after novel cross-linker treatment following a pseudo-clinical approach. Extent of penetration of the cross-linker into the corneal tissues, tensile strength of the cornea and morphometrical analysis of cadaver corneal and keratoconus tissue sections by H&E staining were analyzed. Peptides cross-linked were analyzed by mass spectrometry of separated corneal layers.

Results

The novel chemical cross-linker at the full or 1/8th concentration did not induce apoptosis in the corneal layers as analyzed by TUNEL assay. Cells from the corneal layers of the cross-linker treated cadaver globes maintained their phenotype intact. The cross-linker at either concentration also did not induce any gross morphological changes in the corneal layers of the cadaver as well as keratoconus cornea. Tensile test analysis of the cross-linker treated cadaver and keratoconus cornea indicated that the 1/8th cross-linker treatment induced a better 2.3 fold increase in stiffness by penetratingupto 200 □m into the stroma. Proteomic analysis of the layers of the cadaver cornea treated with the cross-linker has revealed subtle changes in the protein profile.

Conclusions

The novel cross-linker at 1/8th concentration is optimal in increasing the stiffness of the weak cornea and is a promising non-invasive therapeutic agent for treating keratoconus. It is thus suitable for making a formulation in the form of eye-drops for further clinical trials.

O-20

Synthesis of 1, 5-disubstituted Tetrazole Derivatives via a TMS-N_3 Based Ugi Reaction as Anti-cancer Agents and their Docking Study.

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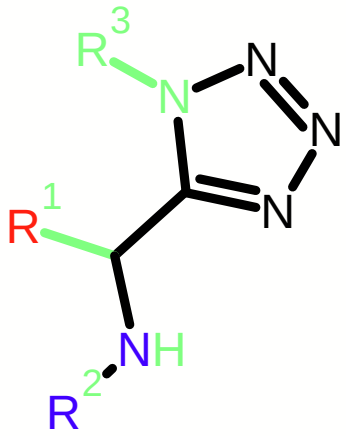
Abstract: In current research scenario, an efficient synthesis has been developed for novel tetrazole scaffolds by single step multicomponent reaction. One of the most promising pathways is Ugi multi-component process for the coupling of four different components in a single reaction step and isolate lead molecule which may serve better life to the society. The syntheses of tetrazoles were undertaken by the Ugi-Multi Component approach with the condensation of aromatic aldehyde containing active pharmacophore, various aryl amines, isocyanide (cyclohexyl isocyanide) and TMS-N_3 under catalyst free reaction condition at room temperature. The structural conformation were carried out by most acceptable spectroscopic technique *i.e.* MS, IR, NMR and single crystal study (XRD) and potency of compounds **(4a to 4h)** were checked at NIH (National Institute of Health) use 60 different cell-lines with respect to nine cancer panels among which compounds **4a** and **4b** have been found to be more potent against different cell lines. On the basis of anticancer data docking was carried out of all the synthesized compounds for their mechanistic study.



Type-1

Keywords: Tetrazole, TMS-N_3, Anti-cancer activity

O-21

Amino acid- Imidazolium Ionic Liquids: Synthesis and Application

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Abstract: Task specific ionic liquids (TSILs) as a catalytic material are growing rapidly in the field of catalysis. Although amino acid ionic liquids were initially introduced as alternative green catalyst/reaction media because of their unique physical and chemical properties and which shows their significant role in controlling the reaction. Amino acid based ionic liquid (AAILs) acidic, basic, or organocatalyst behavior depends upon the functional group attached to the imidazolium. AAILs starting from (S)-proline, have been prepared and evaluated for their ability of a chiral catalyst. The acidic nature of Lewis acidic AAILs as catalysts has been exploited for many organic transformations like tritylation /acetylation of alcohol and phenols. Additionally, the catalyst shows outstanding stability and reusability, and it can be recovered simply and effectively and reused without noticeable loss of the catalytic activity

O-22

tert-Butyl Hydroperoxide as Carbon Source and Hydrogen Ac-ceptor: Regioselective Aminomethylation of Imidazoheterocycles with 2/4-Aminoazaheterocycles *via* Cross-Dehydrogenative Coupling

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Abstract: Transition-metal free construction of C-N and C-C bonds *via* cross dehydrogenative coupling (CDC) reactions represents an ideal strategy in the perspective of green and sustainable chemistry.[1] These reactions generally demonstrate step- and atom-efficiency and eliminate the use of pre-functionalized substrates for C-H bond functionalization.[2] On the other hand, imidazoheterocycles are privileged *N*-heterocycles and have been reported to exhibit a broad range of biological and pharmaceutical properties. The nature of the substituent at the C-2 or C-3 positions of imidazoheterocycles significantly influences the biological activities. More precisely, amido/amino-methylated linkers at C-3 position of imidazo[1,2-*a*]pyridine are found in a number of commercially available drugs such as necopidem, saripidem and GSK812397 for anxioselective activity.[3]

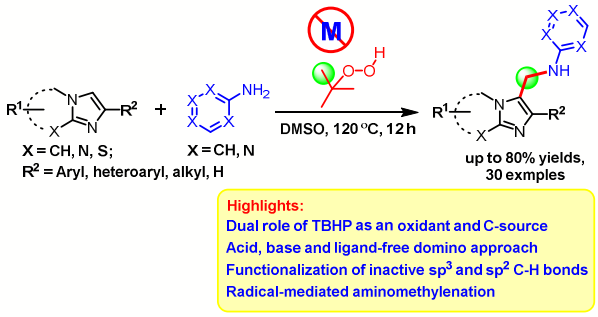

Figure 1. Regioselective aminomethylation strategy

Owing to the valuable application of imidazoheterocycles in drug discovery and our previous work on C-H bond functinalization reactions[4], we herein present a novel, efficient aminomethylation strategy for the regioselective functionalization of imidazoheterocycles with 2/4-aminoazaheterocycles under metal-free conditions utilizing TBHP as a methylene source as well as a hydrogen acceptor. A wide range of imidazoheterocycles and 2/4-aminoazaheterocycles successfully provided corresponding aminomethylated products in moderate to excellent (33-80%) yields. The developed protocol follows radical mediated pathway which is supported by radical trapping experiments and isotopic labelling study.

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O-23

Synthesis, characterization and anticancer activity of Pt(II) and Pd(II) complexes with Schiff base ligands

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Abstract: The transition-metal-based complexes have been explored as a promising delivery vector for cancer therapeutic agents with the potential for great impact on future public health. The platinum metal containing cisplatin is today among the most widely used cytotoxic drug for cancer treatment. The development of transition-metal-based antitumor drug candidates increases the metallopharmaceuticals study dramatically.Platinum-based anticancer drugs, such as cisplatin, carboplatin, and oxaliplatin, are well-established treatment options for a wide range of tumors, particularly in colorectal, testicular and nonsmall cell lung cancers, but they are limited by severe side effects and acquired drug resistance.Hence, the investigation of the anticarcinogenic potential of Schiff base derivatives gains crucial importance. Schiff bases have the capability to bind DNA and proteins, which results in the cytotoxicity of tumourcells[1-7].In this presentation we describe a series of Pt(II) and Pd(II) complexes with bidentate Schiff base ligands. The Pt(II) and Pd(II) complexes have been synthesized by the reaction of metal salts andSchiff base ligands. The compounds were characterized by elemental analyses, melting point determinations, and a combination of electronic, FT-IR, ^{1}H-NMR, ^{13}C-NMR, UV-Vis, mass and X-ray diffraction(XRD) spectroscopic studies. On the basis of analytical and spectral data a square planar geometry may be proposed for Pt(II) and Pd(II) complexes.

The ligands and their metal complexes have been screened against cervical cancer (HeLa) cell lines.Additionally, antimicrobial effects of both the ligands and their complexes on different bacteria and fungi have been recorded. The results are indeed positive. The details of these findings will be discussed.

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O-24

DISTRIBUTION OF VITAMIN D BINDING PROTEIN SUBTYPES IN KUWAITI POPULATION

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Abstract: The vitamin D binding protein (VDBP), also known as group-specific component or Gc, is the major plasma carrier protein of vitamin D and its metabolites. Two single nucleotide polymorphisms have been reported in v*dbp* gene due to missense mutations known as rs7041 and rs4588, which result into three important VDBP isoforms known as Gc1F, Gc1S and Gc2. Significant variations in frequencies of Gc subtypes are reported in different geographical locations. Populations living in northern climates possess more Gc1S and less Gc1F allele. Frequency of Gc2 is much higher in Caucasians and rare in Africans. However, the frequency of Gc alleles is not known in Kuwaiti Population. In this study, 127 healthy Kuwaiti adults were studied for Gc subtypes using molecular methods. Genomic DNA were isolated from the blood of all subjects and the DNA regions covering the targeted mutations were amplified by PCR. The amplified DNA were sequenced and analyzed for specific mutations to determine the Gc subtypes/alleles. The results identified four different Gc subtypes namely Gc1F, Gc1S, Gc2 and GcAin the Kuwaiti population. Among the subtypes, Gc1S (n=106,83.5%) was the predominant, followed by Gc1F (n=80,63.0%) and Gc2(n=47, 37.0%). The fourth subtype, GcA,was the least common allele (n=31,24.4%). The three common subtypes (Gc1F, Gc1S, Gc2), exceptGcA, are well documented in literature. We have identified this variant, namely GcA, due to a missense mutation at rs4588, where threonine is replaced by lysine. The study was supported by Kuwait University Grant No. MM02/17.

O-25

Chemo-enzymatic Synthesis of Modified Nucleosides

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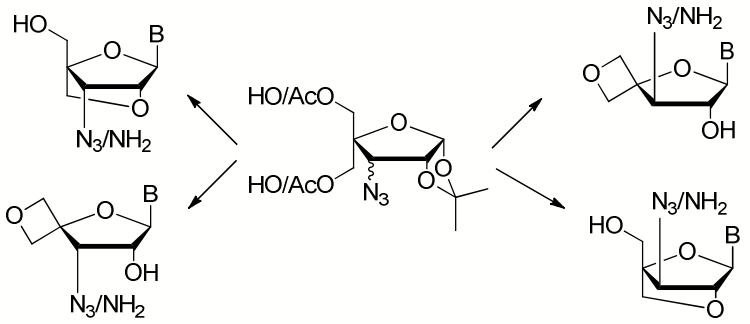
Abstract: Over two decades, a large number of nucleosides have been synthesized, which demonstrated potent antiviral and antitumour activities and have become cornerstones of treatment for patients with cancer or viral infections. Oligonucleotide-based antisense strategies represent a unique paradigm for the treatment of a wide variety of human diseases. In order to discover new class of nucleoside derivatives with enhanced biological activities, the modifications in the sugar moietiy have been attempted, which provide a remarkable level of control over nucleoside sugar puckering and its biological activity.

Herein, we report; (a) the selective biocatalytic acetylation studies on modified 3′-azido-4′-*C*-hydroxymethylated sugar derivatives with an aim to develop an efficient and easy method for the synthesis of *ribo*-azido/amino LNA monomers and *xylo*-azido/amino spiro-oxetano nucleosides and (b) the selective biocatalytic deacetylation studies on modified 3′-azido-4′-*C*-acetoxymethylated sugar derivatives with an aim to develop an efficient and easy method for the synthesis of *ribo*-azido/amino spiro-oxetano nucleosides and *xylo*-azido/amino LNA monomers.



B = Nucleo Bases (T, U, C & A)

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O-26

An Efficient and Sustainable Synthesis of Substituted spirooxindoles via Monoclinic nanozirconia catalyzedMulticomponent reaction of Isatin derivatives with Ethylcyanoacetate and 1,3-dicarbonyl compounds in a Ball mill

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Abstract: These days, the focal point of research is the development of nonhazardous alternatives for the sustainable growth of chemical endeavor that includessolventless organic synthesis, multicomponent reactions, and use of reusable heterogeneous catalysts. Such organic reactions possess various advantages over traditional reactions in organic solvents. They not only reduce the consumption of environmentally perilous solvents but also minimize the formation of other waste material.Subsequently, in recent years, ball milling has emerged as an efficient mechanical method for the grinding of metals and inorganic substances into fine particles. Besidesthe broad applications of ball milling in inorganic synthesis, the potential application and usefulness of ball milling technology as a one-pot, solvent-free route in organic synthesis have largely been overlooked.

A highly efficient, green as well as atom economical protocol for thesynthesis of substituted spirooxindoles from *m*-ZrO2 NPs catalysedmulticomponent reaction of isatin derivatives with ethyl cyanoacetateand 1,3-dicarbonyl compounds in a ball mill has beenestablished. Because of the simple and readily available startingmaterials, easy operation, and high bioactivity of substitutedspirooxindoles, this strategy can be broadly applied to medicinalchemistry. The recyclability of the *m*-ZrO2 Nps catalyst is anotheremphasis of proposed methodology.

O-26

Quercetin, a Natural Flavonoid with Anti-*Helicobacter pylori* Activity,interacts with its Histone-like DNA binding protein: A promising candidate for developing next generation anti-*H. pylori* agents

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Helicobacter pylori (*H. pylori*) infection has strong association with various gastric diseases including gastritis, duodenal/peptic ulcers, and gastric cancer.[1]The pathogen colonizes under harsh acidic and oxidative stress conditions of human gastrointestinal-tract (GI) and can survive there for infinitely longer durations of host life. A recent study demonstrated that histone like DNA binding protein of *H. pylori* –referred here as Hup- serves as akey transcriptional regulator to help the bacterium adapt and combat under acid stress. Additionally, Hup plays an important role in various DNA dependent cellular activities highlighting the importance of this protein as a potential therapeutic target. The *in vivo* activity of Hup can be suppressed by the application of small molecule inhibitorsinterfering the Hup-DNA binding interaction. Working within this framework, the structural and mechanistic investigations have been carried out using solution NMR (Nuclear Magnetic Resonance) spectroscopy in combination with various biophysical, biochemical and bioinformatics methods. The Hup family proteins are known to exist predominantly as a homodimer, however, a recent study from our lab revealed the occurrence of dynamic equilibrium between its monomeric and dimeric conformations.[2] The dynamic equilibrium was found shifting towards dimer both at low temperature and low pH; whereas DNA binding studies evidenced that the protein binds to DNA in its dimeric form. These findings correlated very well with the diverse functionality of the protein and now will form the basis for future studies aiming to develop novel anti-*H. pylori* agents. In our further efforts to perturb the Hup-DNA binding interaction, we are currently exploring the interaction of quercetin with Hup. Quercetin -a naturally occurring flavonoid- has already been shown to reduce the colonization of *H. pylori* and ameliorate the inflammatory response in the gastric mucosa induced by *H pylori*infection. Quercetin is known to interact with DNA[3] and in our molecular docking studies we have also seen its efficient binding in the hydrophobic pocket mapping the dimerization interface **(Fig 1)**. The Quercetin-Hup binding interactionhas been studied in solution using fluorescence quenching as well asNMR based amide chemical shift perturbation methods. Other molecular and cell biology experiments were further performed to evaluate the changes in bacterial morphology and nucleoid structure. Overall, the results clearly evidenced the potential of Quercetin to serve as a precursor candidate for developing promising next generation anti-*H. pylori* agents. The comprehensive outcome of this study will be presented during the conference.

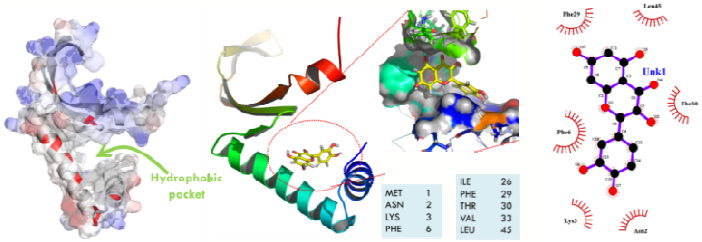

Figure 1: The monomeric Hup structure docked with Quercetin and the Hup amino acid residues involved in binding with Quercetin.

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O-28

Translocation of antibiotics through the outer membrane channel OprE of *Pseudomonas aeruginosa*

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Abstract: Pseudomonas aeruginosa is a significant cause of nosocomial pneumonia and it is the most prevalent pathogen found in patients with severe injuries or burns, where the associated mortality rate is up to 50%. Due to its poorly permeable outer membrane, *Pseudomonas aeruginosa* shows strong resistance to a wide range of antibiotics. Understanding molecular properties of outer membrane channels of these Gram-negative bacteria is of fundamental significance as they are the entry point of polar antibiotics into bacteria. Outer membrane proteomics has revealed OccK8 (OprE) to be among the five most expressed substrate specific channels of the clinically important *Pseudomonas aeruginosa.* The high-resolution X-ray structure and electrophysiology highlighted a very narrow pore. However, experimental *in vitro* methods showed the transport of natural amino acids and antibiotics, among them – ceftazidime, a member of the cephalosporin family. We used molecular dynamics simulations to reveal the importance of the physico-chemical properties of ceftazidime in modulating the translocation through OccK8, proposing a structure–function relationship. As in general porins, the internal electric field favors the translocation of polar molecules by gainful energy compensation in the central constriction region. Importantly, the comparatively narrow OccK8 pore can undergo a substrate-induced expansion to accommodate relatively large-sized substrates

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O-29

Transition metal free chemoselectivesynthesis of isolated and fused fluorenone and study of their photophysical properties

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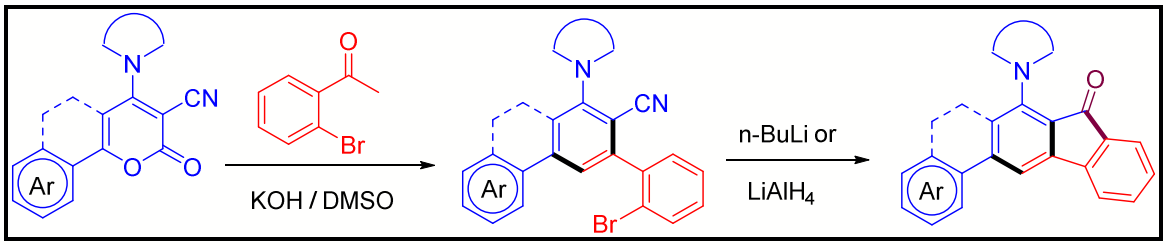
Abstract: Highly functionalized fluorenones was synthesized by chemoselective dehalogenation followed by intramolecular cyclization of functionalized 2"-halo-[1,1':3',1"-terphenyl]-4'-carbonitriles in presence of n-butyllithium or LAH. The required precursor 2"-halo-[1,1':3',1"-terphenyl]-4'-carbonitriles was synthesized by ring transformation of 2-oxo-6-aryl/heteroaryl-4-(sec-amine)-2H-pyran-3-carbonitrileswith o-bromo/chloro/fluoro-acetophenone under basic conditions in moderate yield. Structure of 2"-bromo-[1,1':3',1"-terphenyl]-4'-carbonitrile was confirmed by single crystal X-ray. Photophysical properties of 3-methoxy-7-(piperidin-1-yl)-5H-indeno[2,1-b]phenanthren-8(6H)-one was also explored as this class of compounds are well known for fluorescence.



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O-30

Environmentally relevant concentrations of psychotropic drugsmodify the behavioural patterns of an aquatic invertebrate

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Abstract: Pharmaceutically active compounds (PhACs) are considered as a major contaminants in aquatic environment, having direct and indirect effect on the aquatic organisms even at lower concentrations. This study was aim to assess the effects of methamphetamine and sertraline on the behaviour patterns of clonal marbled crayfish *Procambarusvirginalis*, Lyko 2017. Animals exposed to environmentally relevant concentrations of methamphetamine (~1 µg l^{-1}) did not exhibited significant alteration in distance moved, velocity and activity in presence and absence of available shelters. However, sertraline exposed crayfish were significantly more active in presence and absence of available shelters, while travelled more distance with available shelter than control crayfish. Crayfish exposed to methamphetamine and sertraline spent significantly more time outside the shelters. On the other hand, during exposition of sertraline significantly more crayfish were found with eggs and as dead in the exposed group. Results suggested that the low environmental concentration of PhACs could alter the behavioural and physiological status of crayfish, resulting also in higher reproductive effort and even mortality. These outcomes provide information about possible adverse effect and could assist rapid assessment the ecological consequence of these pharmaceuticals in the aquatic environment.

Keywords: aquatic pollutants, pharmaceuticals, behaviour, *Procambarusvirginalis*, crayfish

O-31

Synthesis of Highly Functionalized Spirobutenolidesvia Nitroalkane Mediated Ring Contraction of 2-Oxobenzo[*h*]chromenes through Denitration

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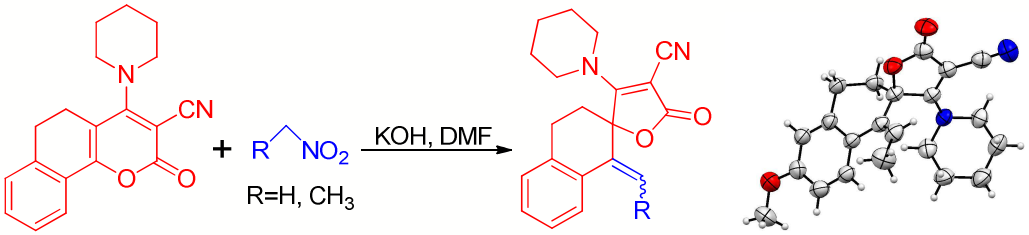

Abstract: Butenolides are a class of lactones, considered as oxidized derivatives of furan with structure made of four carbon heterocyclic ring called furan-2(5*H*)-ones. A broad range of natural products and biologically activitie compounds contain butenolides structural as subunits.[1–3] A facile synthesis of highly functionalized spirobutenolides was carried out through nitroalkane carbanion induced ring opening and relactonizationthorughdenitration reaction of 2-oxo-5,6-dihydro-2*H*-benzo[*h*]chromene-3-carbonitriles. However, when nitroethane was used as a nucleophile source in lieu of nitromethane, a mixture of (*E*)- and (*Z*)-isomer of corresponding spirobutenolideswere obtained in different ratio as evident from proton NMR. The isolated (*E*)- and (*Z*)-butenolides on treatment with sodium ethoxide in DMF at room temperature provided highly substituted trienes via decarboxylation.

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O-32

Synthesis, characterization and biological significance of Cu(II) complexes bearing heterocyclic ligands

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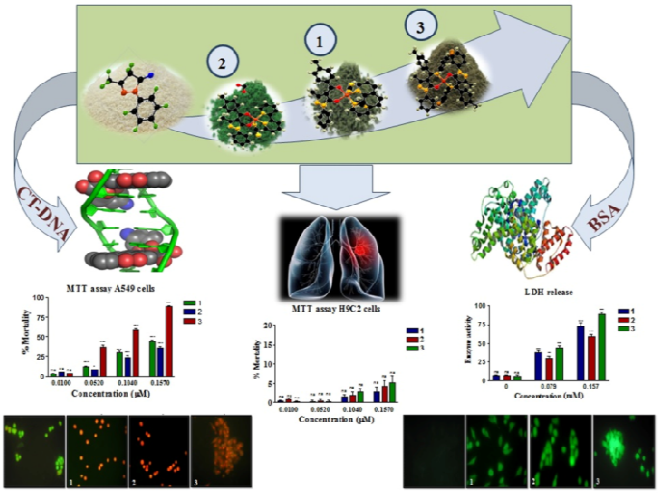
Abstract: Three new 4-acyl pyrazolone based Cu(II) complexes [Cu(TPMP)(Phen)NCS] (**1**), [Cu(TPMP)(Bipy)NCS] (**2**) and [Cu(TPMP-BA)$_2$] (**3**) have been synthesized and characterized by structural, analytical and spectral methods, in order to investigate the influence of ligand substitution on structure and pharmacological properties. In all three complexes, the pyrazolone based ligandsare coordinated to the Cu(II) ion in a neutral fashion as bidentate ligand. The single-crystal X-ray structure of complex (**3**) exhibits a square planar structure, while complexes (**1**) and (**2**) revealed slightly distorted square-pyramidal structures. The interaction of these complexes with Calf-Thymus DNA (CT-DNA) has been explored by absorption and emission titration methods. The interaction of the complexes with bovine serum albumin (BSA) was also investigated using fluorescence spectroscopic method. The results indicated that all of the complexes could quench the intrinsic fluorescence of BSA in a static quenching process. Further, the cytotoxic effect of the complexes **1-3** examined on human lung cancerous cell line (A549) and noncancerous rat cardiomyoblasts (H9C2) cell lines showed that all three complexes exhibited substantial cytotoxic activity. All the pharmacological investigations support the fact that there exists a strong influence of ligand substitution on pharmacological activities.

Keywords: Acyl pyrazolone, Schiff base, Copper complexes, DNA and Protein binding, Anti-cancer activity



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O-33

*In vitro*Anti-hyperglycaemic activity of 4-hydroxyisoleucine derivatives

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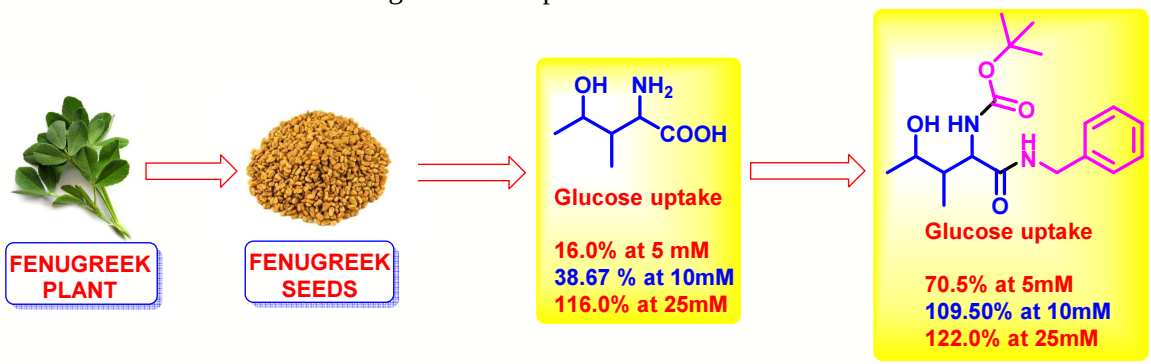
Trigonella foenum-graecum, commonly known as fenugreek or meethi, is an annual herbaceous plant,4-Hydroxyisoleucine, a peculiar amino acid extracted from fenugreek seeds and never found in mammalian tissues, exhibits interesting insulinotropic activity.We isolated the nonproteinogenic amino acid 4-hydroxyisoleucine in large quantity and prepared a series of amides derivatives related tonatural product 4-hydroxyisoleucine and screened their glucoseuptake activity in L-6 skeletal muscle cells. Some of the derivativesexhibited better glucose uptakestimulatory activity than parent compound4-hydroxyisoleucine at 5µM and 10 µM concentrations and two derivatives enhanced translocation of insulin sensitive glucose transporters-4 in skeletal musclecells.



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O-34

Synthesis and Biological Applications of Pyrimidine-based Cationic Amphiphiles

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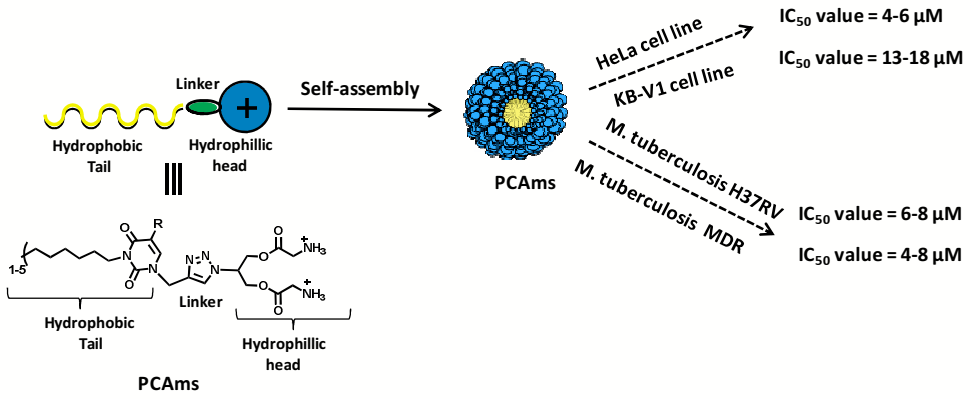
Nano-aggregate have various biomedical applications, such as in cancer and other therapies, drug and in gene delivery, etc. Amphiphilic molecules consists of a core-shell structure having hydrophobic and hydrophilic moieties enhance the solubility of hydrophobic anticancer drugs and facilitates drug loading for delivery purposes. By using cationic amphiphiles (CAms), several drawbacks of traditional chemotherapeutics can be suppressed such as low therapeutic efficacy often caused by poor drug bioavailability and high systemic toxicity. The tumor cells are loosely bound and have leaky blood vessel supply that helps easy entrance of nano-aggregates. Hence the aggregates are delivered more efficiently to the tumor cells. Cationic amphiphiles have been regarded as the safer alternative for viral gene delivery. We have successfully synthesized uracil/thymine based cationic amphiphiles utilizing cheap, commercially available, biocompatible starting materials, *viz.* glycerol, uracil/thymine and glycine. The physicochemical characterization of nano-aggregates in aqueous buffer revealed a trend in their size, zeta potential and CAC. These features appear to have an influence on the anti-proliferative activity of the compounds on the cancer cell line HeLa, its multidrug resistant variant KB-V1, *M. tuberculosis* H37Rv sensitive strain and MDR clinical isolate 591 resistant strain. The detailed synthetic protocol will be discussed during poster presentation.



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O-34

NEW CHROMOGENIC REAGENT FOR HPTLC DETECTION OF ORGANOPHOSPHORUS HERBICIDE GLYPHOSATE IN VISCERAL SAMPLES.

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ABSTRACT

Glyphoset (N-Phosphonomethyl) Glycine or 2- (Hydroxy- oxidophosphoryl) Methyamino)acitie acid) is present the largest selling agrochemical in the world(1)and its market continues to grow in line with the increases in cultivation glyphosate tolerant (GT) Trangenic crops(2).few chromogenic reagent have beenencountered in literature for the detection of glyphosate insecticide by TLC including Dragendorffs reagent, (3) idoplatinate reagent(4), this study reports new method for the analytical determination of glyphosate by TLC method. Chromogenic reagent is sensitive and selective detection of glyphosate after HPTLC is possible. Glyphosate reacts with chromogenic reagent to produce an intence blue colour compound. Presumptive color test for ketamine hydrochloride (5) and cocaine identification on TLC and imidacloprid identification on TLC (6).with this chromogenic reagent have been reported in literature although these method are selective, there are limitation to their use in routine forensic work. Reson to their complex which may damage the columns. And therefore high performance thin layer chromatography is the methods of choice for screening biological sample due to its speed low cost and vesality.

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P-1

Interaction Studies of Catechin Metal Complexes with BSA & DNA using UV-Visible Spectroscopy

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Abstract: Catechins mainly found in green tea have been reported to exhibit a range of therapeutic and toxicological effect against many lethal diseases. Their pharmaceutical actions depend on the interaction of these molecules with biological receptors. In order to identify similar possible ligands of potential medicinal importance and to understand the mechanism of their action, a number of computational tools and instrumental techniques are available. Drug molecules are effectively transported to their targets by albumin protein and DNA is main target for anti-carcinogenic drug molecules. In the present case, UV-visible spectroscopy has been used to identify the interaction of EGCG and EGC metal complexes with bovine serum albumin and DNA. A comparative study has been carried out by calculating the binding constant of these interactions via Benesi-Hildebrand equation. In addition, docking calculations have been performed to investigate the conformational changes which occur during the interaction.

P-2

Pd/PTABS: An Efficient Catalytic System for Synthesis of Base Modified Nucleosides

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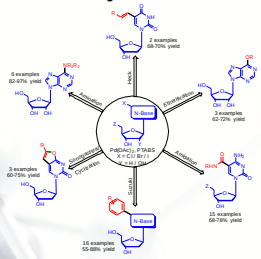
Abstract: Nucleosides hold a large family of natural and chemically modified analogues of a boundless structural diversity and a wide biological activity (Kapdi *et al.* [1]).Modifications interconnected to nucleoside heterocyclic bases have been explored for their potential biological activities like antiviral, antibacterial and anticancer properties. The excellent tuning of palladium catalyst allowsdeveloping the greener and sustainable protocols along with that it also provides the stereo- and regiospecificity by tolerating many functional groups(Shaughnessy*et al.* [2]).Thus, the catalytic potential of palladium precursors can be explored for the development of sustainable methodologies for the modification of nucleosides on the molecular level.

Taking this in consideration, we developed the water soluble and highly efficient palladium catalyst system to carry out the modification of nucleosides. Highly water soluble and versatile catalytic system consisting of palladium acetate and PTABS (7-phospha-1,3,5-triaza-admantane butane sultonate) ligand have been employed for Suzuki-Miyaura, Heck, Sonogashira, amination etherification and carbonyl-amidation under mild set of reaction conditions. The Pd/PTABS catalytic system shows excellent reactivity for Suzuki-Miyuara cross-coupling of halo nucleosides in water as a solvent andallows the column-free isolation of Suzuki-Miyuara cross-coupled product with recyclability of catalytic system. The catalytic system utilized to develop a novel copper-free Sonogashira coupling protocol for the pyrimidine nucleosides has also been established via a one-pot synthesis of FV-100, a nucleoside-based drug in phase 3 clinical trials for herpes zoster treatment. In case of Heck reaction, demonstrated the synthesis of antiviral drug: BVDU (Bhilare *et al.* [3]).This highly efficient catalytic system allows amination of 6-chloropurine with different amines at ambient temperature. The validation of this strategy has been proved via synthesis of uracil based anti-diabetic drug, alogliptin which is an oral anti-diabetic. Additionally, the catalytic system allows the cross-coupling of 6-chloropurine with different phenols offering the corresponding ether product under the mild conditions of reactions. This protocol also applied in the synthesis of XK-469 ester derivative, which is an anti-tumor agent.The same catalytic system was also explored for palladium catalyzed amidation using carbon monoxide gas under fairly mild set of reaction conditions (Bandaru*et al.* [4]).



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P-3

A novel and chemoselective synthesis of 2-arylbenzimidazoles in molecular sieves-MeOH system their antitubercular activity

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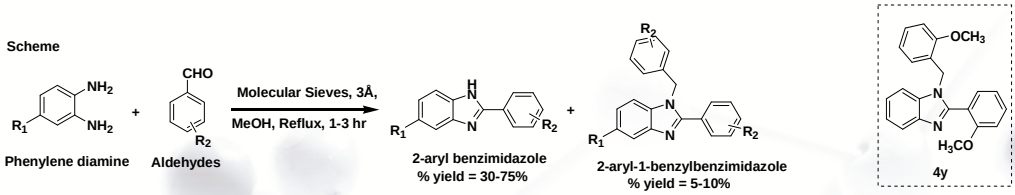
Abstract :

1) Benzimidazole, a biodynamic pharmacophore, is present in several natural products and drug candidates like albendazole and mebendazole as antiparasitics.
2) Being an important pharmacophore several synthetic strategies have been developed, the most common method i.e. substituted 2-arylbenzimidazoles involves the direct condensation of substituted *o*-phenylenediamines with various substituted aromatic aldehydes.
3) Various acidic reagents have been used, such as *p*-TSA, $BF_3.Et_{2O,}$ and Ionic liquids etc. These methods have several drawbacks like lower yields, expensive reagents, longer reaction time and less chemoselectivity etc.
4) We have synthesized chemoselectivity 2-arylbenzimidazoles over 2-aryl-1-benzylbenzimidazoles in terms of an efficient, chemoselective, operational simplicity, economic viability, with greater selectivity and in particular industrial applicability.
5) Molecular sieves used in this reaction are reusable and can be recycled up to three times. Methanol solvent was most suitable for the solution phase synthesis.
6) All these benzimidazole analogues were evaluated against *M. tuberculosis* in BACTEC radiometric assay.
7) The compounds **4y** and **4z** exhibited potential antitubercular activity against *M. tuberculosis* $H_{37}RV$, MIC at 16 µM and 24 µM respectively.
8) Molecular docking results showed that compounds **4y** (−10.2858), and **4z** (−10.5108) docked well with DNA gyrase.
9) The molecular docking results were validated through gyrase supercoiling inhibition assay. Benzimidazoles **4y**, and **4z** exhibited moderate activity against DNA gyrase enzyme.
10) Compound **4y** was well tolerated by Swiss-albino mice in acute oral toxicity up to the dose level of 300 mg/kg body weight. Compound **4y** possessing a diarylbenzimidazole core, can further be optimized for better activity.



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P-4

In silico screening of antibacterial lichen compounds against Xanthomonas oryzae pv. Oryzae

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Abstract: *Xanthomonas oryzae* pv. *Oryzae* (Xoo) is a gram negative bacterium which enters into the root and leaves by way of wounds and cause serious bacterial lead blight (BLB) disease of rice, other grasses, and sedges . BLB disease of rice causes losses of grain yield in world wide. The main symptoms of BLB disease are wilting of seedlings, yellowing and drying of *leaves. Currently many types of chemicals use to control Xoo bacteria which cause environmental pollution and also affect human health. Hence* there is a need to discover new drug which can obtained from natural source and can be effective for the treatment against Xoo bacteria. Therefore we conducted virtual screening of a library of 200 compounds of lichen against Peptide Deformylase protein as a receptor of Xoo bacteria. The results showed that the compounds of lichecn namely ; Pulvinamide, Evernic acid, Sativic acid, Acetylportentol, Russulfoen and N ostoclide II have batter negative binding energy with Peptide Deformylase as compare to reference molecule. The range of molecular binding energy obtained from docking study were -10.8 kcal/mol to -7.8 kcal/mol comparing reference molecule Ampicillin (-7.6 kcal/mol). Hence we conclude that these lichen compounds can be used as drugs against Xoo bacteria.

Key word- *Xanthomonas oryzae* pv. *Oryzae*, Lichen**,** Virtual Screening, bacterial lead blight (BLB) disease.

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P-5

Potassium persulfate promoted N-nitrosation of secondary and tertiary amines with nitromethane under mild condition

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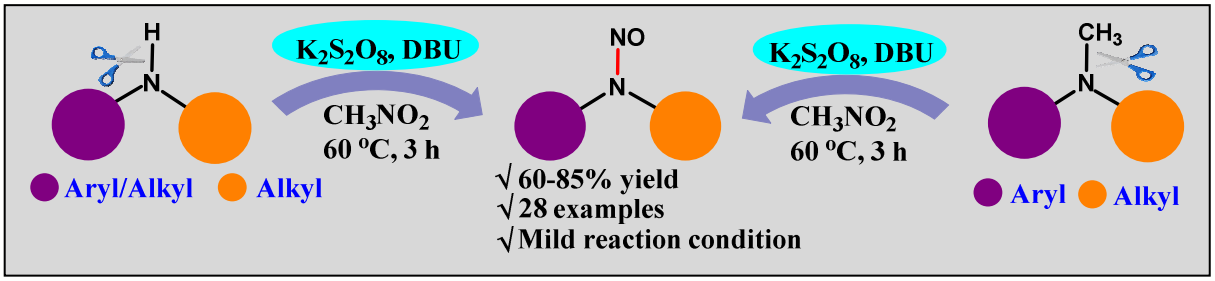
Abstract :*N*- Nitrosamines are versatile class of organic compounds that received continuous interest in biochemical research due to their unique carcinogenic and mutagenic properties. On the other hand, *N*-nitrosamines play an important role in organic synthesis as starting materials, masking groups, directing groups etc. For example, synthesis of hydrazines, nitramines and sydnones were typically achieved from corresponding *N*-nitrosamines. In addition, recently *N*-nitroso functionality has been emerged as a traceless directing group for various metal catalyzed aryl C-H functionalization reactions.

A simple and efficient route for the N-nitrosation of various secondary amines with nitro methane is described in the presence of potassium persulfate and DBU. Under optimized condition, tertiary amines underwent a dealkylative N-nitrosation with good yields. Inexpensive reagents, broad substrate scope and efficient conversion make the current protocol more attractive in organic synthesis.



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P-6

Concise Asymmetric Syntheses of (2*R*,3*S*)-3-Hydroxyproline and (2*S*,3*S*)-3-Hydroxyproline

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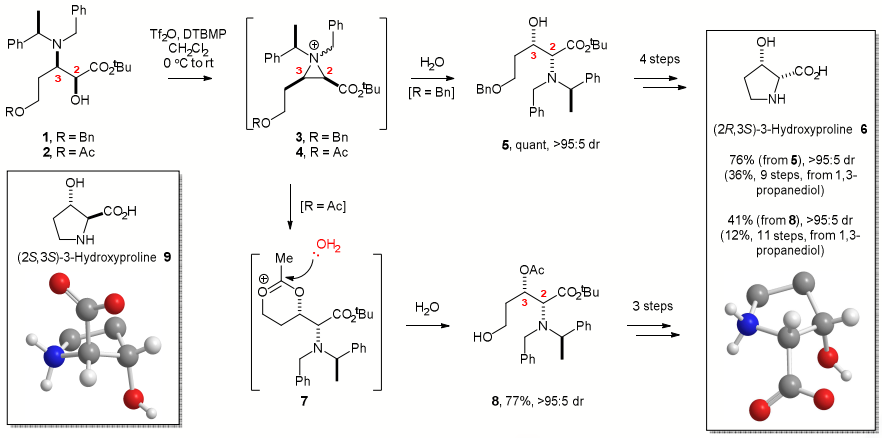
Abstract : Two synthetic routes have been developed for the asymmetric syntheses of (2*R*,3*S*)-3-hydroxyproline **6**. (2*R*,3*S*)-3-Hydroxyproline **6** and its C(2)-epimer (2*S*,3*S*)-3-hydroxyproline **9** have been isolated from a diversity of natural sources, including hydrolysates of the antibiotic telomycin,[1] and collagen of varied origin.[2]The key step in both synthetic strategies is the conversion of protected α,δ-dihydroxy-β-amino esters into protected β,δ-dihydroxy-α-amino esters, via the intermediacy of the corresponding aziridinium ions.[3] Activation of the C(2)-hydroxy moieties within **1** and **2**(derived from 1,3-propanediol in 47% and 55% in 3 and 4 steps, respectively) as the corresponding triflates followed by displacement by the amino group results in the formation of aziridinium species **3** and **4**. Regioselective ring-opening of **3** with H_2O gave β-hydroxy-α-amino ester **5** in quantitative yield. Intramolecular ring-opening of **4** via a tethered nucleophile (i.e., an acetate group) gave acetoxonium ion **7**, and hydrolysis of **7** resulted in exclusive formation of β-acetoxy-α-amino ester **8** in 77% yield. α-Amino esters **5** and **8** were then cyclized and deprotected to afford (2*R*,3*S*)-3-hydroxyproline **6**, from commercially available 1,3-propanediol, as a single diastereomer (>95:5 dr) in 36% and 12% overall yields, respectively. The C(2)-epimer (2*S*,3*S*)-3-hydroxyproline **9** has also been synthesised via both inter- and intra-molecular aziridinium opening in 5.5% and 26% yields, respectively.[4]



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P-7

Visible-light Photoredox Catalyzed Synthesis of Carbocycles

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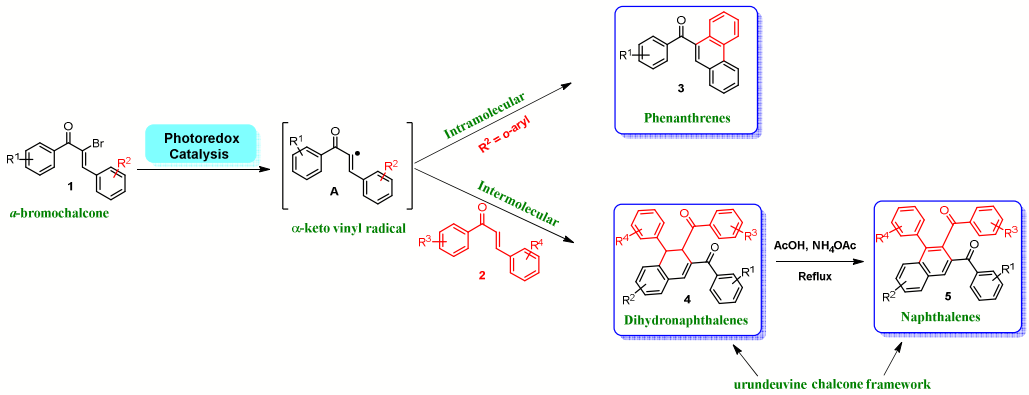
Abstract : Recently the use of visible light to develop greener synthetic protocols has attracted the attention of the chemist's community, since the visible light is not only abundant, it is also an environment friendly and greener alternative to the conventional chemical synthesis. MacMillan *et al*. [1]. Visible-light photoredox catalyzed inter/intramolecular cyclizations have been established as a versatile tool for the synthesis of various polycyclic scaffolds. Reiser *et al.* [2]. We employed *α*-bromochalcones for the generation of *α*-keto vinyl radicals via an oxidative quenching cycle of the iridium complex under visible light photoredox catalyzed conditions. These radicals were trapped inter- or intramolecularly for the synthesis of carbocyclic scaffolds such as phenanthrenes **3**, Rastogi *et al.* [3] and dihydronaphthalenes **4,** which were conveniently oxidized to the corresponding naphthalenes **5** Rastogi *et al.* [4]. The later protocol was adopted successfully for synthesizing derivatives of urundeuvine chalcones.



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5. Savita B. Nagode,[a,b]Ruchir Kant,[c]and Namrata Rasto

P-8

Metabolic and Lipidomic Profiling of Oral Squamous Cell Carcinoma in Tissue Specimens using ^{1}H HRMAS MR Spectroscopy

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Introduction: Oral squamous cell carcinoma (OSCC) represents more than 90% of all head and neck cancers. *Ex vivo* ^{1}H HRMAS NMR studies of oral tissue specimens had identified predictive biomarkers in order to understand the malignancy induced biochemical perturbation for early cancer detection (Srivastava, Roy et al. 2011).

Materials and Method: ^{1}H HRMAS MR Spectroscopy and its corresponding chemometric studies on OSCC and corresponding non-involved tissue have been performed on 182 tissue specimens obtained from 52 patients. Metabolic perturbations were profiled by subjecting NMR data to multivariate analysis using 'The Unscrambler X' software packages. Perturbations in lipid compositions measured using univariate Box-Whisker plot.

Results: Representative NMR spectra of malignant tissues shows decreased fatty acids and lipids and significantly increased glutamate, glycine, lactate, taurine, choline containing compound and alanine. The classification of malignant tissue from benign tissue set was observed with more than 95% sensitivity. Further a significant reduction of triglycerides (TG) amount observed in malignant tissues with higher free fatty acid (FFA) fractions.

Conclusion: Our study revealed that multiple tissue samples during oral cancer surgery are required for exploring the full potential of magnetic resonance spectroscopy metabolic profiling. Such approach may provide higher potential in defining the prognosis of the patient.

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P-9

Defection: A route for antibiotic resistance in mycobacterial population

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Abstract : Drug resistantmycobacterial populationhave been declining the antibiotic treatment fficacy and causing mortality(1).Mycobacterial population(s)develop resistance to antibiotics through different mechanisms. One of the mechanisms, we propose, is"Defection". In simple terms,this can be defined as unwillingness to carry out an act.In biological terms, it can be defined as alteration of expression of one or more related proteins that are directly or indirectly involved in mediating the activity of antibiotic and making the cell resistant to that antibiotic.

In this study we have attempted to understand the virulence potential, cross resistance,and immune responses of mycobacterial population selected against antibiotics Pyrazinamide (PZA) and Ethambutol (ETB).These antibiotics are first line drugs used in the treatment of Tuberculosis (TB) caused by the *Mycobacterium tuberculosis* (*M.tb*). The *Mycobacterium marinum* is a close relative of *M.tb*and shows ~85% sequence similarity with it(2).*M. marinum* causes TB like disease in fish and amphibian

*M.marinum*is gradually selected in the increased concentration of PZA and ETB.In every concentration, three rounds of selection have been performed.Growth kinetics have been noted during selection process. The antibiotic selected mycobacterial population showed growth inhibition and SDS page analysis exhibited differential protein expression.Mouse tail vein injectionof antibiotic selected *M. marinum* retained their virulence in-vivo. All these data suggest that “Defection” might be a route adopted by the mycobacterial population to acquire resistant over antibiotics

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P-10

Design, Synthesis and Biological Evaluation of Novel Molecules for The Management of Alzheimer's Disease

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Abstract : Alzheimer's disease (AD) is chronic neurodegenerative disorder characterized by loss of neurons in the hippocampal region of the brain. In India approximately 4.1 million are suffering from dementia. This is going to be tripled by 2050 if no successful drug comes into the market. Although the pathophysiological of AD is not yet completely known however, there are several literature evidences including publications from our group indicating the key role played by acetyl and butyryl cholinesterase, Aβ aggregates, metals and oxidative stress in the neurodegeneration in AD. Currently available drugs in the market for AD focused on symptomatic relief for the initial few months. Natural products have gain enormous interest for the treatment of AD. Ferulic acid has shown promising neuroprotective property, however, it suffers from several drawbacks such as it exhibits weak interaction with cholinergic system, low logP value and poor water solubility. To develop naturally inspired multifunctional neuroprotective molecules, we embarked on the development of Ferulic acid (FA) analogs. FA is connected to heterocyclic amines via suitable 2 or 3 carbon linker. We have successfully synthesized, characterized and carried out biological evaluation of the developed novel molecules. The lead molecules F2 has shown *in-vitro* acetylcholine esterase inhibitory studies (IC_{50}=2.74 uM, vs < 20% inhibition at 20µM by FA. F2 is also able to quench free radical in DPPH assay and chelate metal in UV based experiments. F2 will be tested for Aβ aggregation modulation activity. The detailed studies will be presented

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P-11

New ionic Cu(II) and Co(II) DACH–flufenamate conjugate complexes: spectroscopic characterization, single X–ray studies and cytotoxic activity on human cancer cell lines

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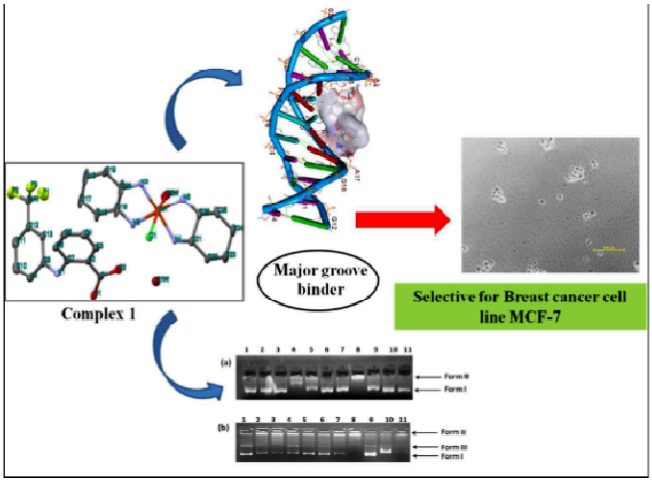
Abstract: New ionic [{M(DACH)$_2$(H$_2$O)Cl}.(fluf)] [where M = Cu(II), Co(II)] antitumor drug entities **1** and **2** were prepared and characterized by spectroscopic studies and single X–ray crystallography. Preliminary *in vitro* binding studies of **1** and **2** with ct–DNA have been carried out by biophysical methods which revealed electrostatic binding mode of these drug entities with ct–DNA preferably by external surface or groove binding mode contrary to other NSAIDs drugs which show intercalative binding. Comparative EPR titrations of complexes **1** and **2** alone and in presence of ct–DNA were performed to validate the mode of binding which revealed that there was no significant change in EPR spectra of complexes alone and complexes incubated with ct–DNA implicating that coordination geometry of metal ions does not alter. Validation of antitumor potential of **1** and **2** was done by cytotoxicity experiments against human cancer cell lines by SRB assay. Complex **1** was active against all tested cell lines with an exceptionally low GI_{50} value = 2.9 µg/ml against MCF–7 cell line showing its preferential selectivity. On the contrary, conjugate **2** showed poor activity against all tested cancer cell lines.



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P-12

Rationally designed peptide based cancer nanotherapeutics

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Abstract: Harnessing self-assembled peptides for generating nanostructured material posses a great promise in delivering toxic conventional small molecule drugs and nucleic acid based biopharmaceuticals for developing cancer nanotherapeutics. Clinically safe intracellular delivery of cargo in functional form remains a major concern for the pharmaceutical industries. We aim to engineer peptide based therapeutics for intracellular functional drug delivery and developing combination therapy for breast cancer treatment. We have evaluated gramicidin (gA) and gA-inspired hydrophobic peptide (LD8) for delivering doxorubicin (Dox) and TAT-peptide inspired arginine-rich cell penetrating peptides for intracellular delivery of functional siRNA to silence critical oncogenic pathways. Both gA and LD8 induce cytotoxicity, mitochondrial depolarization and apoptosis against MDA-MB-231. Doxorubicin loaded LD8 (LD8-Dox-NP) and doxorubicin loaded gA (gA-Dox-NP) showed cytotoxicity and apoptosis, evidenced by DNA fragmentation and Western blot analysis of PARP cleavage and upregulated tumor suppressor protein p53, that inhibits cell proliferation. gA-Dox-NP and LD8-Dox-NP induce S and G2 phase cell cycle arrest, respectively, indicating inhibition of DNA synthesis by gA-Dox-NP and DNA damage in presence of LD8-Dox-NP. gA-Dox-NP and LD8-Dox-NP can be potentially used as 2-in-1 nanomedicine in treating breast cancer. Our designed arginine-rich molecular transporters demonstrated functional siRNA delivery in MDA-MB-231 cell line like commercial transfection agent HiPerFect and showed significant gene silencing in upregulated MAPK/ERK signaling pathway in breast cancer, evidenced by RT-PCR and immunofluorescence studies. We are also examining these against pathways upregulated in drug resistance, metastasis and epithelial-mesenchymal transition.We anticipate such therapeutic peptides might be translated to clinics for developing advanced siRNA based nanotherapeutics, combination therapy in breast cancer treatment and silencing signal transduction of oncogenic pathways can emerge as unique paradigm in developing cancer nanomedicine.

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P-13

Role of EspH: Essential for virulence but ineffective to elicit protective response

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Abstract: The emergence of phenotypically variant forms in isogenic members of a clonal cell populationrenders fitness advantage and facilitates the survival in continually changing environments with the help of natural selection of abest suited strategy(1). Phenotypic noise is defined by the variation in the level of protein expression among the different isogenic members of a clonal cell population sharing common environment(1). We have characterized noisy expression of numerous proteins in the *Mycobacterium marinum*wild-type population with varied functions. Among them, the Rv3867 (EspH) is an extended RD1 region protein which is indirectly or directly involved in the regulation of Esx-1 secretory apparatus. It also regulates the expression of another protein TlyA that function as an inflammatory molecule. Therefore, to ascertain the role of Rv3867 in *M. marinum* infection, the Rv3867 immunized mice were challenged with *M. marinum*WT population (2). It is observed that the Rv3867 immunization isnot able to elicit protective response in *M. marinum*wild-type infected mice. While, the virulence symptoms have enhanced to an extent that suggests that the immunization is worsening the pathology at least in the acute phase of infection. Possibly the noisy expression of Rv3867 protein might help the bacterium in balancing the expression of phenotypes responsible for virulence.

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P-14

Early repair salivary biomarkers in post-periodontal surgery by NMR metabolomics: A proof of concept

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Abstract: Oral microflora is a well-orchestrated and sequential defense mechanism for any infection related to oral disease. Chronic periodontitis is a disease of microbial challenge to symbiosis and homeostasis. Periodontal surgery is the most promising cure with repair process in periodontal regeneration. It has encouraging outcome in terms of early biomarkers. Saliva of periodontal surgery subjects with the chronic periodontitis have been evaluated by ^{1}H NMR spectroscopy in search of possible early metabolic differences that could be obtained in order to see the eradication of disease that favors symbiotic condition. The study employed 176 saliva samples in search of distinctive differences and spectral data were further subjected to multivariate and quantitative analysis. The ^{1}H NMR study of periodontal surgery samples shows clear demarcation and profound metabolic differences as compared to the diseased condition. Several metabolites such as glutamate, lactate, ethanol and succinate were found to be of higher significance in periodontal surgery in contrast to chronic periodontitis subjects. These could be considered as early repair markers for chronic periodontitis as they are being restored to achieve symbiosis. The study therefore concluded early recovery process of diseased subjects with restoration of possible metabolomic profile similar to the healthy controls.

P-15

A visible light mediated synthesis of benzimidazole molecules utilizing carbon nitrides as photocatalyst

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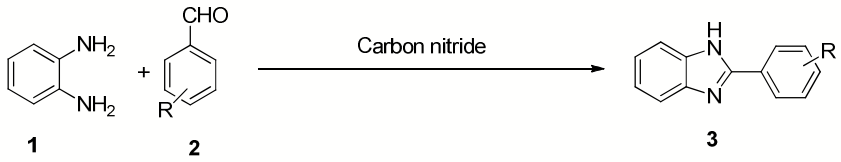
Abstract: Although the first synthesis of benzimidazoles was reported in 1872 by F. Hoebrecker, it was in the decade of 1950's when its biological significance was discovered. Since then benzimidazole molecule containing structures have been an integral part of various pharmaceutical, agro-chemical and veterinary products. They have varied biological activities like anti-cancer, fungicidal, analgesic, bactericidal, proton-pump inhibitor, anti-viral etc. Thus, compounds having benzimidazole motif have been used widely in medicinal chemistry and in drug development, hence researchers are always pursuing new methods for facile synthesis of benzimidazole motif. During the last few decades, synthetic organic chemistry has seen a paradigm shift from conventional methods to "greener" ways of synthesis. These include the use of non-toxic reagents, reusable catalysts, mild reaction conditions etc. Herein we are reporting an environmentally benign and efficient method for synthesis of benzimidazole molecules by visible light radiation using graphitic carbon nitrides as photocatalyst. Carbon nitrides are already established as an efficient photocatalyst for organic transformations. The reaction proceeds smoothly under mild conditions and affords good to excellent yields of product, the catalyst can be easily separated and reused in further reaction cycles. This convenient and user-friendly approach can expand the use of graphitic carbon nitrides in organic synthesis.



Scheme 1.

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P-16

MycobacterialOutliers:Are they a trade-off between abundance and significance?

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Abstract: Outliers areentities that do not fit into the realm of the group from they were identified. In biology, outliers refer to the organisms or cells that show a behavior or trait, different from their related population. Biological outliers often discarded from analysis either in form of their exclusion from statistical studies to get smooth statistical patterns or their masking through the analysis techniquesthat studies phenotypic impact by mean expression level studies.Thus, outliers have always been subjected to discrimination for their likely biological significance owing to their low abundance in the population. However, the advancement in single cell analysis techniques and appreciation for the need of studying population behavior in appropriate environmental context, outliers are being recognized and appreciated for their biological significance. This essentially indicates that the statistical significance should not be used as a sole read-out to analyze the biological meaning.

We have characterized an outlier population in *Mycobacteriummarinum* in terms of surface localization of an inflammatory protein, TlyA(1). Considering the potential inflammatory role of TlyA protein in mycobacterium, the noisy surface expression of this protein can likely be reasoned as a result of fitness bound optimal limits to its costly expression. Our initial attempt to understand the likely role of TlyA surface expressing outlier population in population fitness involves the enrichment of TlyA defectors without any deliberate endogenous or ectopic genetic manipulation. Our initial observations are quite interesting and stimulating that we look forward to present in the conference.

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P-17

Three component one pot synthesis 6-amino-2-pyridone-3,5-dicarbonitrile derivatives using piperidine base ionic liquid as an efficient catalyst

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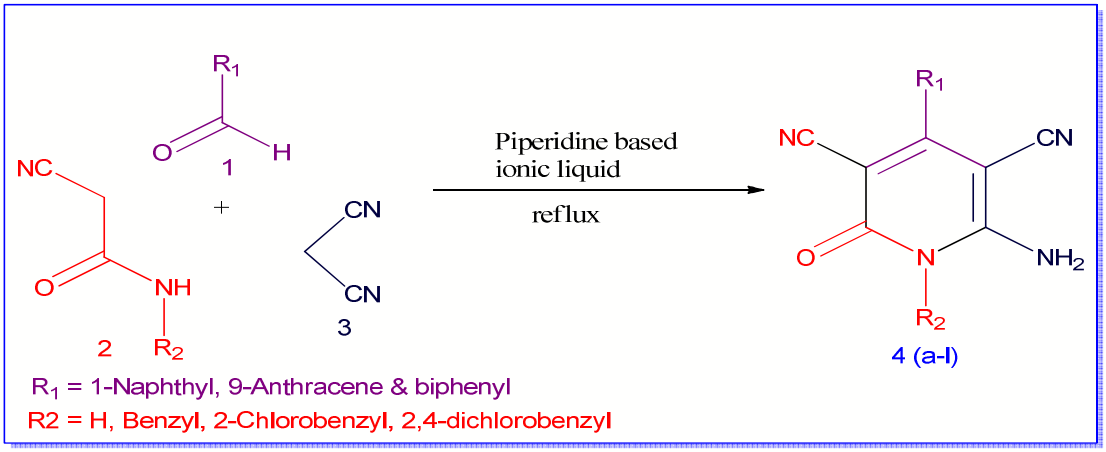
Abstract: In this study, we reportsimple and convenient method for synthesis of 6-amino-2-pyridone-3,5-dicarbonitrile derivatives from various aromatic aldehydes, malononitrile and cyanoacetamide and its derivatives via one-pot synthesis. Reported reaction is efficiently catalyzed via piperidine based ionic liquid.Structures of the newly synthesized compounds were confirmed by various spectroscopic methods.A characteristic property of this reaction includes the excellent yield (79-88%), shorter reaction time and ease of product isolation.



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P-18

A New Avenue to the Synthesis of Chromeno[2,3-*d*]pyrimidine-trione Derivatives Catalysed by Lemon Juice: Methyl Arenes as Sustainable Surrogates of Aryl Aldehydes

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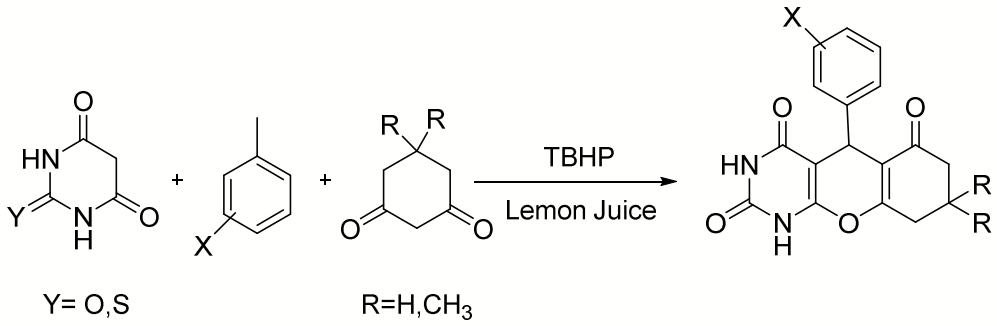
Abstract: In the perspective of green chemistry, multi-component reactions (MCRs) are found to be growing technique in organic synthesis as it shows remarkable significance in construction of diverse and complex organic molecules in a single event which includes all essential parts of the starting materials.In addition, several advantages such as eco-friendly nature, less time consumption, superior atom economy,simple purification process, minimum waste disposal etc. makethem extremely useful in synthetic chemistry.In recent years, environmentally benign synthetic methods have received considerable attention and some green protocols have been developed. There has been a large emphasis both in the chemical industry and in academic research for the synthetic utility of natural catalyst in organic transformations. Nitrogen, oxygen and sulphur containing heterocyclic compounds have received considerable attention due to their wide range of pharmacological activity.In view of the above point, fruit juice of Citrus limon (lemon juice) has been utilized as a natural and renewable and biodegradable catalyst for the green and environmentally friendly preparation of Chromeno[2,3-*d*]pyrimidine-trionesformulti-component reaction of barbituric/ thiobarituric acid, 1,3-diketones and methylarenes as precursors of aryl aldehydes. Aryl aldehydes were generated *in situ* by oxidation of methylarenes with tert-butyl hydroperoxide (TBHP).



Scheme: Synthesis of Chromeno[2,3-*d*] pyrimidine-triones

P-19

A Redox-based Superoxide Generation System using a Quinone Reductase of *Escherichia coli*

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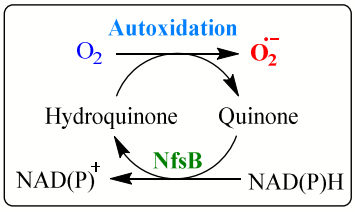
Abstract: Superoxide generation under physiological conditions is the key to understand its biochemical role in living systems. Despite many chemical and enzymatic systems being presently used for this purpose, there is a need for an alternate, cheap and robust system for superoxide generation. [1] Xanthine/xanthine oxidase is the only enzymatic system that has been widely applied for *in vitro* biochemical studies. Although, it suffers from limitations such as low substrate solubility, its irreversible consumption, and the lack of a heterologous expression system for xanthine oxidase. [2] We report a redox-based, enzyme-driven system, in which superoxide is generated by the autoxidation of hydroquinone to quinone (Q) *via* semiquinone. [3] The hydroquinone level is maintained by NfsB, a quinone reductase (QR) of *Escherichia coli* strain K-12 [4] that reduces quinone to hydroquinone in presence of NAD(P)H. We coupled the Q/QR with glucose/glucose dehydrogenase system to aid ample supply of NAD(P)H. We used the hydroethidine probe to detect and quantify the generation of superoxide using NMR and HPLC. Among various quinones tested, menadione emerged as the optimal substrate for superoxide generation under optimized conditions. The newly developed system relies on the recyclable quinones with relatively superior water solubility, as well as heterologously expressed enzymes. This redox-based system presents a viable alternative for studying the biochemistry of superoxide under different physiological and pathological conditions. [5]



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P-20

A zwitterionic Zn(II) benzothiazole nanohybrid conjugate as hydrolytic DNA cleavage agent

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Abstract: An organic–inorganic hybrid protonated zinc–benzothiazole complex, $[Zn(C_{14}H_{13}N_4S_2)Cl_3]$ (**1**) has been synthesized which crystallizes in triclinic *P1* space group possessing the lattice parameters, a = 7.949(5) Å, b = 10.076(5) Å, c = 11.810(3) Å, α = 80.654(5)º β = 89.667(5)º, γ = 70.095(5)º per unit cell [1]. Each $[Zn(C_{14}H_{13}N_4S_2)Cl_3]$ unit is connected to the neighboring molecule by intermolecular hydrogen bonds between the apical chlorides and amine nitrogen atoms resulting in a one–dimensional chain–like arrangement. DNA interaction studies of **1**were performed by employing different spectroscopic studies depicting groove binding mode with partial intercalation, enunciated by molecular docking studies [2,3]. The quantitative analysis of intra and intermolecular non–covalent interactions were also carried out using Hirshfeld surface calculations to explore H–bonding and C–H/π interactions [4]. Transmission electron microscopy (TEM) analysis of the zinc−chlorido complex demonstrated the particle size in the range of 40−70 nm. The hydrolytic pathway of **1** with pBR322 plasmid DNA was substantiated by cleavage activity in presence of ROS scavengers which exhibited significant cleavage of supercoiled form to nicked form in presence of hydroxyl radicals [5]. More evidence for hydrolytic mechanism mediated by zinc–benzothiazole hybrid complex was obtained by DNA religation experiment using the T4 ligase enzymeand the kinetic aspects of the mechanism followed are also discussed.

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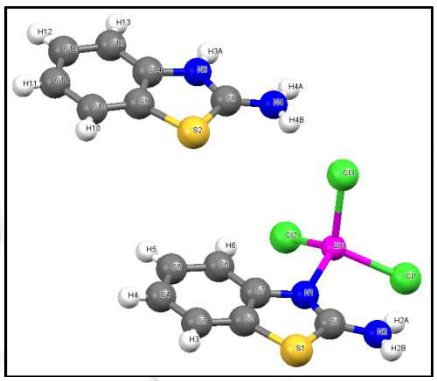

Fig.ORETP view of complex **1**.

P-21

Design and synthesis of new chiral copper-(II) sulfa drug based 1D coordination polymers; DNA binding, cleavage and SOD mimetic activity.

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Abstract: New chiral smart Cu(II) 1D coordination polymers**1a** and **b** were synthesized from the reaction of Schiff base with sulfa drug as ancillary ligand. Structure elucidation was done*via* different spectroscopic and single X-ray crystal diffraction studies.The complexes crystallized in the monoclinic P21 space group, possessing the lattice parameters a = 12.2577(15) Å, b = 4.9211 (6) Å, c = 20.538(3) Å, α = 90 °, β = 98.225(5) °and γ = 90 °in complex **1a** and a = 12.3189(9) Å, b = 4.9315(4) Å, c = 20.6308(15) Å, α = 90 °, β = 98.288(3) ° and γ = 90 ° in complex **1b** per unit cell, respectively.Interaction studies of **1a** and **b** with ct−DNA were carried out employing different biophysical studieswhich revealed that the L-enantiomer of Cu(II) complex, **1a**, binds more strongly than the D-enantiomer. *In vitro* superoxide dismutase activity of redox active complexes was evaluated by using a xanthine/xanthine oxidase-NBT assay which demonstrated excellent SOD mimicsfor L-enantiomer compared to D-enantiomer (IC_{50} values 0.106 and 0.19 μM, respectively).Furthermore, molecular modeling studies were carried out to appreciate molecular features important for drug–enzyme interactions which offer new insights into the experimental model observations.

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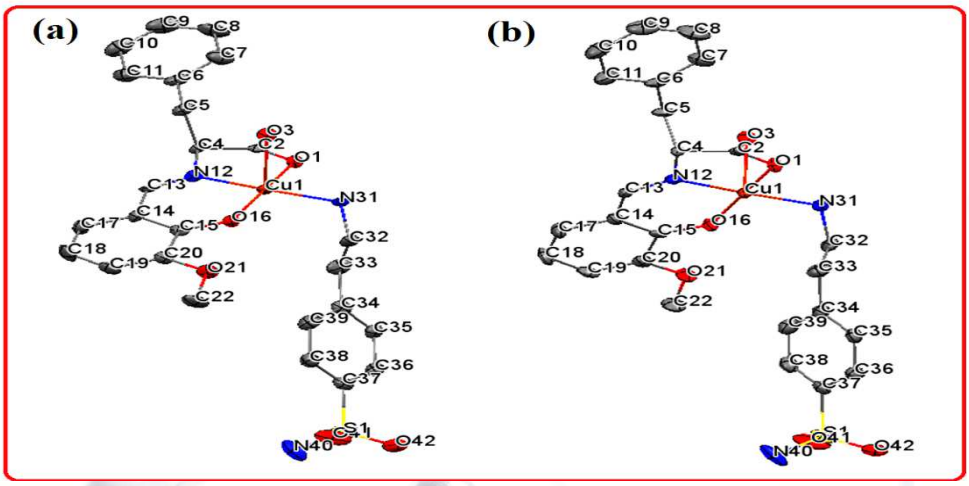

Figure: Structure of complex (a) **1a** and (b) **1b.**

P-22

[3+3] Cycloaddition for heterocyclic synthesis via *insitu* generation of azomethine ylide as Dipolar adduct.

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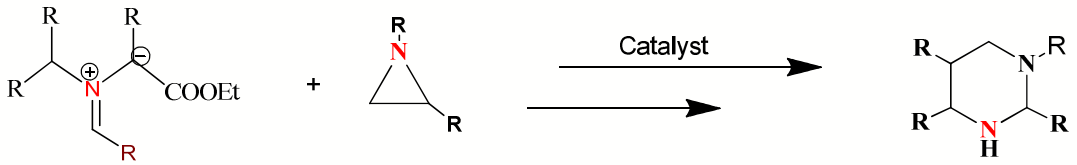
Abstract: The synthesis of hexahydropyrimidine derivative is always been a tough task for scientists. Hexahydropyrimidines derivative compounds are biological active compounds and they are found in many natural products[1]. Many derivatives of hexahydropyrimidine shows important role in biological activities like antibacterial[2], antitumor, and anti-inflammatory activities[3] etc. Here, we have developed a very efficient way of synthesis of hexahydropyrimidine derivative by using aziridine and azomethine ylide via [3+3] cycloaddition. occurring as concerted or stepwise process. Cycloaddition reactions are among the most useful synthetic constructions in organic chemistry. Of these transformations, the concerted [4+2]- cycloaddition, the Diels- Alder reaction, is by far the best known and most widely applied. However, although symmetry disallowed as a concerted process and lacking certifiable examples until recently, stepwise [3+3]- cycloadditions offer advantages for the synthesis of a substantial variety of heterocyclic compounds, and they are receiving considerable attention.



R= Aliphatic and Aromatic

Scheme 1

Reaction takes place at ambient temperature. Operational simplicity, environmentally, economically and biologically viable,and [3+3]-cycloaddition is crucial features of this protocol.

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P-23

GRAPHENE OXIDE-CATALYSED GREEN APPROACH FOR AMINATION OF AROMATIC/ALIPHATIC RINGS VIA NITRENE INSERTION ON ACTIVATED C-H BOND .

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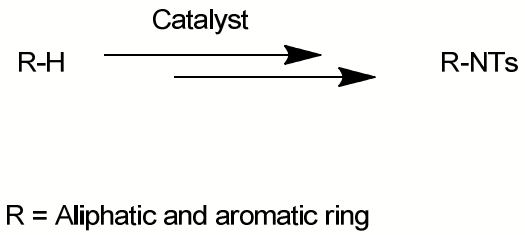
Abstract: The C-N bond formation is a topic of current interest among scientists. Various strategies for C-N bond formation have been developed in past decades . Nitrene transfer reaction catalysed by metal based catalysts on saturated and unsaturated substrates makes an important methodology in organic synthesis.[1,2] Aziridine ring formation takes place upon addition of nitrene moiety on unsaturated substrate where as C-N bond formation takes place in case saturated substrate by insertion of nitrene moity into C-H bond. [3] Graphene oxide also have the property for C-H activation.[4]Here we are interested in nitrene insertion into C-H bond by green approach using water as solvent, I_2, PhINTs as nitrene sourse, and grapheme oxide as a catalyst. By using this system we have synthesized aminated products..



Scheme 1

Reaction takes place at ambient temperature. Operational simplicity , no side product, environmentally viable, atom economy, reusability of grapheme oxide, are crucial features of this protocol.

References:

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P-24

Colorimetric and Fluorogenic Detection of Toxic Hydrogen Sulphide Gasin Biological Medium by Metal-Organic Framework

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Abstract: Hydrogen sulfide (H_2S) has been recently recognized as one of the three important biosynthetic gasotransmitters including nitric oxide (NO) and carbon monoxide (CO). Thus, H_2S can function as a signal transmitter in living organisms. This gas, which is endogenously generated by enzymes, is engaged in regulating a variety of important genes. Owing to its considerable role in biological systems, the detection as well as controlling the levels of H_2S in highly demanding for investigating and better understanding of its physiological and pathological functions.Numerous fluorescent turn-on probes for the sensing of H_2S have been reported so far in the literature based on the above concern.

The dinitro-functionalized Zr(IV)-based metal-organic framework (MOF) material namely DUT-52-$(NO_2)_2$ (**1**, DUT = Dresden University of Technology) was successfully employed as a fluorescent turn-on probe for the detection of H_2S under physiological conditions. The compound displayed naked-eye colorimetric responses towards H_2S under daylight as well as under UV radiation with a detection limit of 20 μM. The probe **1'** is capable of sensing H_2S in blood plasma and in mouse macrophage J774A.1 cells.The unprecedented selectivity for detection of H_2S even in the existence of other potentially competing biomolecules and in biological system makes the presented compound a potential candidate for the real-time monitoring of H_2S in biological systems.

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P-25

A Metal-Organic Framework Showing Highly Selective and Sensitive Detection of Exogenous and Endogenous Formaldehyde

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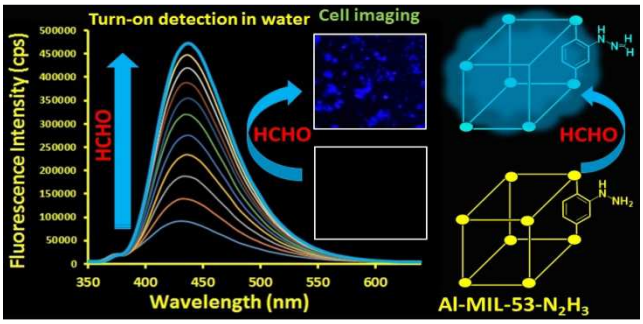
Abstract: We report a new hydrazine functionalized Al(III) metal-organic framework (MOF) having MIL-53 (MIL = Material of Institute Lavoisier) framework topology for the sensitive and selective detection of formaldehyde (FA). The phase-purity of the thermally activated and as-synthesized forms of the material was examined by X-ray powder diffraction (XRPD) experiments, Fourier transform infrared (FT-IR) spectroscopy and thermogravimetric (TG) analysis. The desolvated material (**1′**) showed great potential for the selective sensing of FA in the existence of other potentially competitive aldehydes in both aqueous and 10 mM HEPES buffer (pH = 7.4) media. The fluorescence "turn-on" behavior of the reaction-based probe can be ascribed to the inhibition of photo-induced electron transfer (PET) process (from hydrazine group to phenyl ring) due to the formation of hydrazone moiety. The detection limit towards FA for the probe in HEPES buffer is 8.37 µM (0.25 ppm), which lies below the intracellular concentration of FA (100-400 µM). A very short response time (1 min) has been displayed by **1′** for FA sensing. Moreover, a remarkable enhancement in the emission intensity (7 fold and 4 fold in aqueous and HEPES buffer medium, respectively) of **1′**was observed after 1 min of FA addition. Furthermore, the ability of the probe to detect FA in the vapor phase was demonstrated. Interestingly, the material is also capable to detect endogenous FA in cancer cells. All the above discussed features clearly reveal that the present material has a huge potential for selective recognition of FA in both real water and biological samples.



Scheme 1. Schematic representaion of sensing behaviour of the MOF formaldehyde

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P-26

Surviving in cold: White adipose tissue adaptations

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Abstract: Cold adaptation in mice (that maintain a constant body temperature of 37° C), is a high energy demanding situation requiring sustenance of metabolic rate much higher than basal. Long-term cold adaptation recruits several mechanisms for survival in mice including increased insulation, behavioral modulation (hurdling and curdling), shivering and activation of nonshivering thermogenesis (NST). For many decades, Brown adipose tissue (BAT) was been considered as the only site of NST in mice. However, studies of past decades have shown that white adipose tissue (WAT) and skeletal muscle also serve as alternate sites of NST and can be recruited to a higher level upon special needs. It has been suggested that adipocytes inside WAT acquire BAT-like properties (called browning) and start to produce heat for body temperature maintenance. But, WAT being the primary sites of lipid storage are tapped during high energy demand like that of cold in animals. So, from a classical stand point we can propose that WAT undergoes lipolysis and provide free fatty acid to be used by/in other NST sites like skeletal muscle and heart. Towards this hypothesis we have tried to gain insight about several different WAT depots and their differential adaptation during long-term adaptation to mild (16 °C) and extreme (4 °C) cold. We have employed UCP1-KO and SLN-KO mice to decipher the role of inguinal WAT, which has been speculated to be important for browning. Our studies support in favor of the classical interpretation.

P-27

SCAFFOLD SHIFT FROM PYRANONE CARBOXAMIDE TO PYRAZOLYL ACETAMIDE

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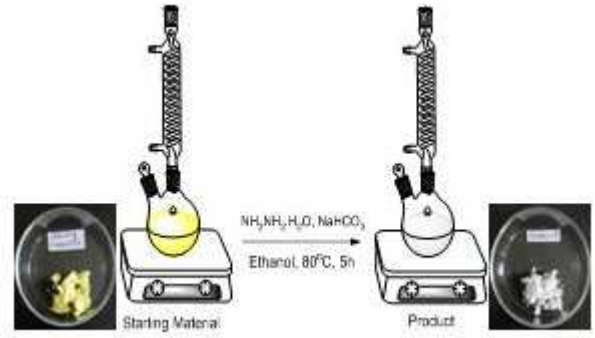
Abstract: An efficient intramolecular ring transformation strategy was developed for the synthesis of substituted pyrazolyl acetamide using hydrazine. The product obtained can be formed using two paths one is intermolecular attack and other is intramolecular cyclization. To study the mechanism, all structures were optimized using DFT/B3LYP method using Gaussian and the mulliken charges of each atom of optimized structure were calculated. Using this, intramolecular path is confirmed via intermediate (4-hydrazinyl-pyranone carboxamide). All structures were confirmed using spectroscopic technique LCMS, UV and NMR.



Keywords: *pyrazolyl acetamide, intra-molecular,* DFT, B3LYP, Mullikan charges, NMR

P-28

Role of Ca2+-entry mediators in muscle during adaptation to cold

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Abstract: Recent studies have provided insight on role of "Skeletal muscle" as a site of non-shivering thermogenesis (NST), in addition to relatively better known phenomena of shivering during cold adaptation. For the performance of NST, the muscles undergo several structural as well as biochemical changes. Cold induced NST leads to reorganization of muscle sarcoplasmic reticulum (SR) and mitochondria-SR positioning. The SR serves as a Ca2+-store in the muscle and ryanodine receptor (RYR) 1-mediated leak of SR-Ca2+ has been focus of several studies as a mechanism. However, role of RYR1-independent Ca2+ signaling in the muscle cells has not been studied so far. Studies have demonstrated that Ca2+-channels on the plasma membrane also influence many Ca2+ signaling pathways inside the muscle. This process is called Ca2+ entry by proteins like STIM1, Orai1 and TRPC1. Therefore, we have analyzed the expression profile of key Ca2+ entry proteins of skeletal muscles during cold exposure. Our studies demonstrate that levels of Ca2+ entry proteins are altered during cold adaptation, revealing pathways that may play more fundamental physiological role than expected in skeletal muscle.

P-29

Conditionally Essential Target for anti-tubercular drug discovery

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Abstract: Discovery of the four regimens –Isoniazid, Rifamycin, Pyrazinamide, and ethambutol was a significant breakthrough in tuberculosis (TB) management. Unfortunately bacterium's resilient nature andits ability to adopt a quick latent state have resulted in rapid development of drug resistance. TB has come out as the leading cause of death from a single infectious disease. Novel drug discovery scenario currently focusing on the particular drugs that are active against resistant, dormant, and latent bacteria has been acknowledged till date. Pretomanid, Bedaquiline and Delamanid discovery in recent date heal the situation against multi drug-resistant and extensively drug-resistant TB. When we deeply observe the mechanism pattern of newer as well as established one; they all are acting upon "Essential Targets" of bacteria. Quick resistanceagainst essential proteins shifted the focus towards "Conditional Essential protein" – mycobactin synthetase complex, which express only at a particular stress condition in host body for the survival of pathogen. Targeting this protein can give an alternative significant platform as "Conditionally essential target approach" in tubercular drug discovery.

P-30

Targeting muscle metabolism to counter the "Syndrome X"

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Abstract: Metabolic syndromes including obesity and type II diabetes are becoming more and more common all over the world. These phenotypes broadly have been labeled as "Syndrome X". It is widely accepted that this trend is due to dysregulation of energy homeostasis in an individual. In an animal body, energy enters in the form of food and exits as work and heat. The body tries to store unspent energy which activates several metabolic remodeling of various organs, which is a major cause of initiating the program leading to the metabolic disorders. Muscles undergo remarkable remodeling during the progression events of Syndrome X. Interestingly; muscle is also shown to be a site of adaptive thermogenesis. Therefore, it is possible that mechanisms contributing to adaptive thermogenesis in muscle can be targeted to increase whole body energy expenditure providing protection against Syndrome X. One of such mechanism is sarcoplasmic reticulum Ca2+-ATPase (SERCA)-mediated ATP utilization which is regulated by several factors like sarcolipin, SR-lipid composition, myoregulin. Towards identification of SERCA-activators, here we have analyzed the literature to shortlist small molecules that are known to activate muscle metabolism such as capsaicin, AICAR, ephedrine, caffeine. We have obtained preliminary results that capsacin enhances sarcolipin-binding to SERCA leading to increased ATP usage. Our next, goal is to understand the mechanism how the shortlisted muscle activators work. We anticipate such studies will facilitate fragment-based approach to better target SERCA function.

P-31

Synthesis and NMR studies of α-Pyranonecarboxamide analogs

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Abstract: Hepatitis C virus shows very high genetic variability, moreover they are becoming drug resistant and current mechanisms show side effects. These issues demand newer scaffoldings for promotion of alternate mechanisms. Hereby we report the discovery of a new pyranone carboxamide scaffold with n-methyl piperazine as a prospective anti-HCVagent. Comprehensive NMR study of n-methyl piperazine α-pyranone carboxamide shows a distinguishedcoupling peak for H_a, and $H_e$due to conformational locking. The conformational studies were delineated in detail to demonstrate 3D structure features of the compound.

P-32

SYNTHESIS AND X-RAY STRUCTURAL STUDIES OF NOVEL PYRIDINONE ANALOGS

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Abstract: The synthetic route for the intramolecular ring transformation of pyranone carboxamide to pyridinone has been optimized. The scheme for the reaction depicts the role of base in ring transformation. The catalytic effect of bases like NaH, 1-methylpiperazine and Acetamidine on pyranone carboxamide lead to the characterization of three different products.On reaction of pyranone carboxamide with NaH(base) in THF(solvent), resulted in the formation of decarboxylated product. 1-methylpiperazine functions as an organic base and transforms the pyrano carboxamide into pyrdinonecarboxylate. The reaction of pyranone carboxamide catalysed by acetamidine results in the formation of pyrdinone carboxylic acid. The significance of the methodology is the intramolecular ring transformation by simple base catalysis andcost-effective method to get pyridinone class of molecules. The compounds were characterized by ^{1}H NMR and structure studies were carried out using single crystal X-ray studies.

P-33

Synthesis of 4'-methyl-6'-methylene carbocyclic nucleosides

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Abstract: Introduction of 4'-methyl and 7-deaza base were chosen to improve the medicinal chemistry properties in final carbocyclic nucleosides. The newly synthesized carbocyclic compounds were designed for antiviral activity against Hepatitis B Virus (HBV).Among the synthesized compounds, some of themexhibited interesting anti-HBV activity. The carbocyclic sugar construction mediated by BINAP-rhodium catalyzed reductive carbocyclization of 1,6-enynes followed by asymmetric hydrogenation.Mintsunobu reaction was utilize to install 7-deazaadenine analog as bioisostere of adenine base to yield novel carbocyclic nucleoside.

Keywords: Reductive carbocyclization,Mitsunobu reaction, Aristeromycin, Entecavir, Carbocyclic nucleoside.

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P-34

Synthesis and crystal structural studies of isoxazol-3-yl-acetamide derivative

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Abstract: The scaffold transformation of pyranonecarboxamide by treating with hydroxylamine hydrochloride yielded the desired isoxazolyl-acetamide derivative. Hydroxylamine efficiently substituted the thiomethyl group present in the pyranone-3-carboxamide.Following which intramolecular attack of oxygen at C-6 carbon that attacked at the carbon bearing has been replaced efficiently using and sodium bicarbonate. Further, the hydroxyamino carboxamide cyclizes into five membered ring as a result of rearrangement.X-ray quality single crystal of isoxazolylacetamide was prepared by using methanol as solvent for crystallization. Non-covalent interaction studies were conducted to understand the packing of isoxazolyl acetamide.

P-35

Role of aromatic-aromatic interaction in functioning of transcription factors

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Abstract: Almost all physiological processes and cellular adaptations are mediated and modulated by involvement of various transcription factors leading to change in levels of important functional proteins. Transcription factors recognize their specific response elements upstream of a gene on the DNA thereby leading to modulation of mRNA levels of specific genes. Different physiological conditions utilize specific transcription factors to mediate the cellular signaling processes. For the binding of the transcription factor to the recognition DNA element intra-protein, protein-protein and DNA-protein interaction contribute. In many proteins that act on nucleic acids, aromatic-aromatic (AA) interactions play key role in the DNA-protein binding. Therefore, we hypothesized that AA interaction might be critical for bridging the contact points between the DNA response element and residues of the transcription factors. If this is true, such AA interactions may serve as the determinants of the recognition events between DNA and the transcription factors. Using literature-based approach, in-silico mutagenesis and molecular dynamics (MD) simulations we have investigated various AA interactions in 5 different transcription factors. Our studies highlight the fact that AA interactions are critical in establishing the early contact points and these pockets may be targeted to inhibit the actions of transcription factors.

P-36

Cytokines as potential recruiters of adaptive metabolism

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Abstract: There are two well-described non-shivering thermogenic (NST) sites; brown adipose tissue (BAT) and skeletal muscle (SKM), each utilizing distinct mechanisms of heat production. Mitochondrial metabolism is the molecular basis of thermogenesis in BAT, while it plays minor role in SKM. Here, we wanted to document changes in mitochondrial ultrastructure in these two tissues upon adaptation to mild (16°C) and severe (4°C) cold in mice. At thermoneutrality (29°C), mitochondria in both the tissues were loosely packed with irregular cristae. Adaptation to severe cold showed most dramatic remodeling of mitochondrial architecture; even mild cold initiated ultrastructural remodeling of mitochondria including acquisition of more elaborate cristae structure in both thermogenic sites. Also we report cold-induced upregulation in levels of humoral factors: FGF21, IL1α, PYY, TNFα, and IL6 and downregulation of both insulin and leptin. In summary, adaptation to cold leads to enhanced mitochondria function in the SKM and BAT. Further, this study indicates that circulating cytokines might play an important role in the synergistic recruitment of the thermogenic program including crosstalk between SKM and BAT. Understanding the operation of NST mechanisms in SKM and BAT may provide pharmacological targets to increase whole body energy expenditure to counter metabolic diseases.

P-37

Nucleic Acid Binding Studies of Synthetic β-Carboline Derivatives: Spectroscopic Approaches to Derive a Model of the Drug: Nucleic Acid Complex

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Abstract: The β-carboline alkaloids are a large group of natural and synthetic indole alkaloids that possess a common tricyclic pyrido[3,4-b]indole ring structure [1, 2]. Theyare commonly present in plants, animals andsome are formed naturally in the biological system [3].These compounds are of great interest due to their diverse biological activities including sedative, anticonvulsant, antitumor, antiviral, antiparasitic, antileishmanial, antifungal, antioxidative as well as antimicrobial activities [4-7]. The proposed drugs have been reported to possess significant antileishmanial activities [8]. In this study fluorescence was employed to evaluate the binding of three β-carboline derivatives (named 14d, 14f and 14t) with CT-DNA, yeast-RNA and transfer-RNA. All compounds 14d, 14f and 14t illustratesa strong fluorescence emission peak at333nm, 324nm and 337nm. The decrease in fluorescence maxima intensity was observed in all the cases by the addition of nucleic acids which confirmed the binding of the proposed β-carboline derivatives with nucleic acids. The binding constant for all the nine complexes (14d:CT-DNA, 14d:y-RNA, 14d:t-RNA, 14f:CT-DNA, 14f:y-RNA, 14f:t-RNA, 14t:CT-DNA, 14t:y-RNA, 14t:t-RNA) was calculated using double reciprocal plot method and the obtained binding constants are $4.5x10^6M^{-1}$, $9.2x\ 10^5M^{-1}$, $3.3x10^6M^{-1}$, $1.6x10^7M^{-1}$, $6.0x10^6M^{-1}$,$1.6x10^6M^{-1}$, $1.2x10^6M^{-1}$, $3.6x10^5M^{-1}$ and $1.5x10^5\ M^{-1}$ respectively. The binding constant values clearly demonstrate that all complexes provideexcellent binding with nucleic acids. On comparison of binding constants of all complexes it was revealed that 14f:CT-DNA showed maximum value of the binding constantamong all the complexes.

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P-38

A green solvent for synthesis of glucocorticoids prodrugs: DFT approach

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Abstract: In the present work we used Ionic liquids (ILs), N-methylpyrolidone hydrogen sulphate, ([NMP]HSO_4) as green catalysts for the synthesis of biologically active methylprednisolone prodrugs **2** and **3**. The prodrugs were synthesized by coupling of non-steroidal anti-inflammatory drugs such as indomethacin and mefenamic acid with methylprednisolone [1] through esterification using ionic liquids ([NMP]HSO_4) [2]. The ionic liquid was recycled and was reused for further synthesis. The structure of prodrugs was characterized with the help of ^1H, ^{13}C NMR, FT-IR and mass spectrometry. Density functional theory (DFT) studies were also carried out using Gaussian 09 program package for prodrugs **2** and **3** using B3LYP/6-31G (d, p) basis set [3]. Vibrational frequency calculated for compounds **2** and **3** at the same level, where the vibrational frequencies were scaled down by 0.9608 [4] scaling factor. The ^1H and ^{13}C chemical shifts were calculated with the GIAO method [5]. Electronic properties such as HOMO-LUMO energies were measured with the help of time dependent DFT method. From the global reactivity analysis we conclude that the prodrugs **2** exhibited greater global electrophilicity index value (3.5915 eV in case of chloroform), suggests that it can behave as a good electrophile as compare to **3**. On the basis of first hyperpolarizability, **2** (9.068×10^{-30} esu) showed, good attractive materials for non linear optical (NLO) application. An important feature of the present synthesis is that two important anti-inflammatory drugs have been conjugated together
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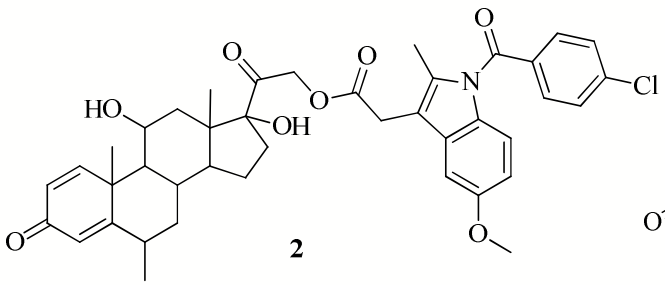
Keywords: methylprednisolone, prodrug, N-methylpyrolidone hydrogen sulphate, global reactivity, NLO.



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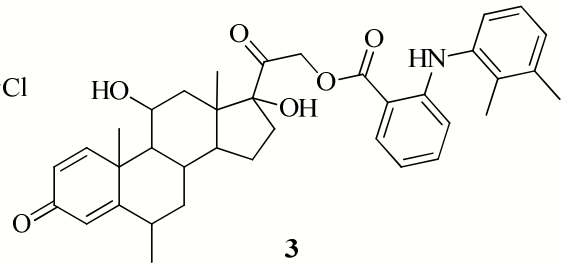

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P-39

Facile synthesis of a series of novel pregnane derivatives and its glycosides

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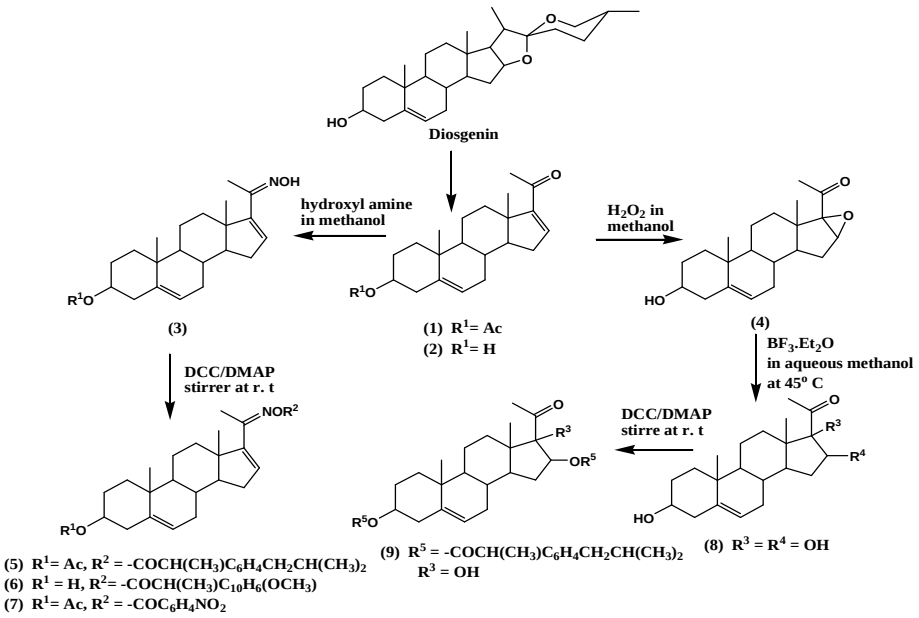
Abstract : Pregnane, the C-21 steroidal derivatives have been dynamically studied and they have been found to possess vast varieties of pharmacological activities like anti-inflammatory (A. Nobile et al. [1]), anti-asthmatic (Y. Shen et al. [2]), anti-feedant (K. K. Purushothaman et al. [3]) and anti-cancer (M. Iqbal Choudhary et al. [4]). A series of novel pregnane derivatives were synthesized from 16-dehydropregnenolone acetate (**2**), obtained by degradation of naturally occurring plant product-diosgenin (A. Sethi et al. [5]). Some novel oxime esters (**5**), (**6**) and (**7**) were synthesized by reaction of oxime (**3**) with NSAIDs like Ibuprofen, naproxen and p-nitro benzoic acid respectively. Epoxide (**4**) was opened by $BF_3.Et_2O$ in aqueous methanol yielding product **8**. The compound **8** on Steglich esterification with NSAIDs like Ibuprofen afforded compound **9**. A novel pregnane glycoside (**14**) was also synthesized. The synthesized compounds have been characterized with the help of spectroscopic techniques like ^1H, ^{13}C NMR, FT-IR, UV-vis spectroscopy and ESI-MS.



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P-40

A green protocol for synthesis of cholesterol prodrug using Ionic liquid: A DFT approach

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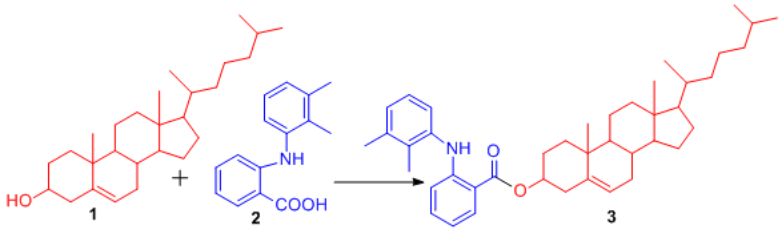

Abstract: In the present research work chloest-5-en-3β-yl-2-((2,3-dimethyl phenyl)amino)benzoate (**3**) has been synthesized in high yield by the reaction of cholesterol (**1**) with non-steroidal anti-inflammatory drug 2-[(2,3-dimethylphenyl)amino]benzoic acid (**2**) using ionic liquid N-methylpyrolidone hydrogen sulphate, ([NMP]HSO_4) as a green catalyst [1]. The characterization of synthesized compound has been done by ^{1}H, ^{13}C NMR, FT-IR, UV-visible spectroscopy and mass spectrometry and 2D NMR (HSQC and HMBC). DFT studies were carried out using density functional method (DFT/B3LYP) with 6-31G (d, p) basis set [2]. A UV-visible spectrum of the synthesized compound was recorded and TD-DFT was applied to calculate electronic properties such as frontier orbitals and band gap energies. Intramolecular interactions have been identified by **AIM** (atom in molecule) approach [3]. The reactivity and reactive site within the synthesized prodrug was examined with reactivity descriptors (global and local). The molecular electrostatic potential (MEP) surface analysis has also been carried out. Dipole moment, polarizability and first static hyperpolarizability were calculated for this steroidal prodrug, which suggests that this prodrug could find use as potential non-linear optical material.

Keywords: cholesterol, ionic liquid, esterification, DFT.

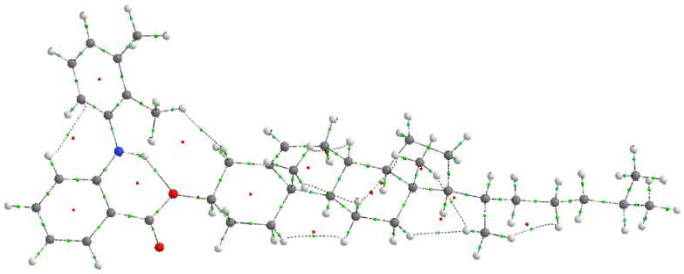

Fig:1 Molecular graphs of synthesized compounds using AIM program at B3LYP/6-31G

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P-41

Use of ionic liquid in the synthesis of pregnane derivatives

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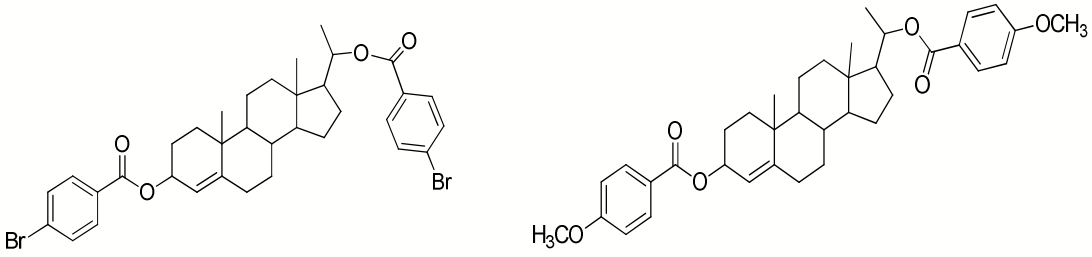
Abstract : Reduction of Preg-4-ene-3, 20-dione [1,2] with sodium borohydride in methanol at 0ºC yielded a 20-hydroxy derivative, which on esterification with p-bromo benzoic acid and p-methoxy benzoic acid (anisic acid) in chloroform yielded compound B and C respectively. Esterification by Steglich procedure [3] leads to the formation of by-products and the solvent and catalysts used are lethal for environmental health. Thus keeping environmental safety in mind Esterification was carried out in presence of 'Ionic liquid' $[NMP]HSO_4$ as a catalyst [4]. The structure of the product formed was confirmed by ^{1}H NMR, ^{13}C NMR, UV, IR techniques. DFT studies were carried out using density functional method (DFT/B3LYP) with 6-31G (d,p) basis set [5]. A UV-Visible spectrum of the synthesized compound was recorded and TD-DFT was applied to calculate electronic properties such as frontier orbitals and band gap energies. Intramolecular interactions have been calculated by DFT method. The reactivity and reactive site within the synthesized pro-drug was examined with reactivity descriptors (global and local). The molecular electrostatic potential (MEP) surface analysis has also been carried out. Dipole moment, polarizability and the first static hyperpolarizability were calculated for this pregnane derivative.

Keywords: Pregnane, steglich esterification, ionic liquid, reactivity descriptor, TD-DFT, MEP



Compound B Compound C

Pregnane derivatives from ionic liquid

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P-42

"Regioselective Azidation of Alkenes using Sulfonium Iodate Reagent"

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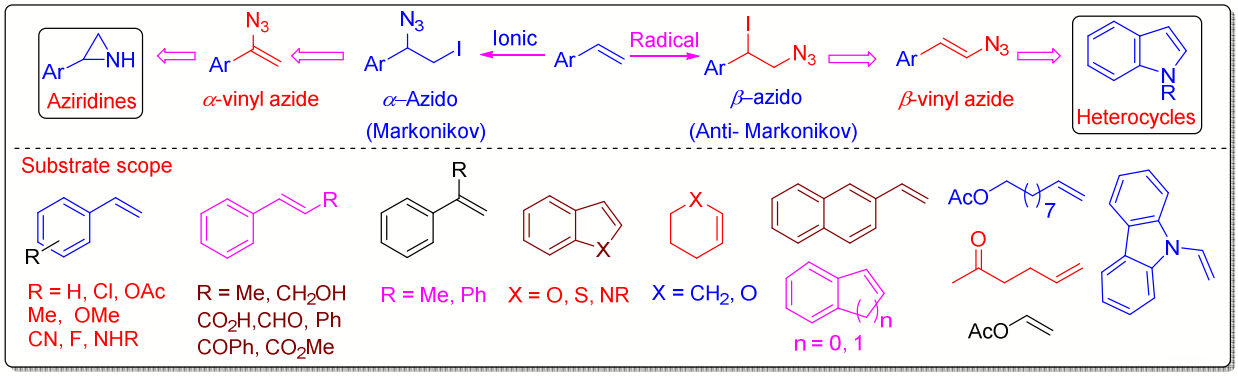
Abstract:1,2-Bifunctionalization of olefins by the selective addition of azide and iodo groups are important chemical transformation in organic synthesis. The resulting azides can readily be transformed into versatile intermediates such as vinyl azides, amines, aziridines, tetrazoles, etc., which display antituberculosis, antibiotic, anticancer, immunostimulating, and *anti*-HIV activities.[1-3]In addition, with the development of "Click Chemistry", various organic azides arerequired as starting materials for producing 1,2,3-triazoles possessinga wide spectrum of biological activities.[4,5]

In this context, we developed a novel reagent system for regioselective azidation of alkenes, the combination of $Me_3SI(OAc)_2$andNaN_3 has been found to be an efficient, simple and inexpensive metal free reagent system for 1,2-bifunctionalizationof alkenes.[6,7] Sulfonium iodate reagent promoted the iodoazidation ofalkene providingα-azidoiodo derivatives through ionic mechanism (Markonikov addition), whereas β-azidoiodo compounds were obtained when the reaction proceeds *via*radical mechanism (*anti*-Markonikov addition).A variety of synthetically useful functional groups are compatible with our mild reaction conditions. This protocolenables the straightforward synthesis of various functionalized azides in good yields.



$Me_3SI(OAc)_2$ promoted regioselective azidation of alkenes.

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P-43

MacMillan Catalyst as an organocatalyst for the Asymmetric Biginelli Reaction

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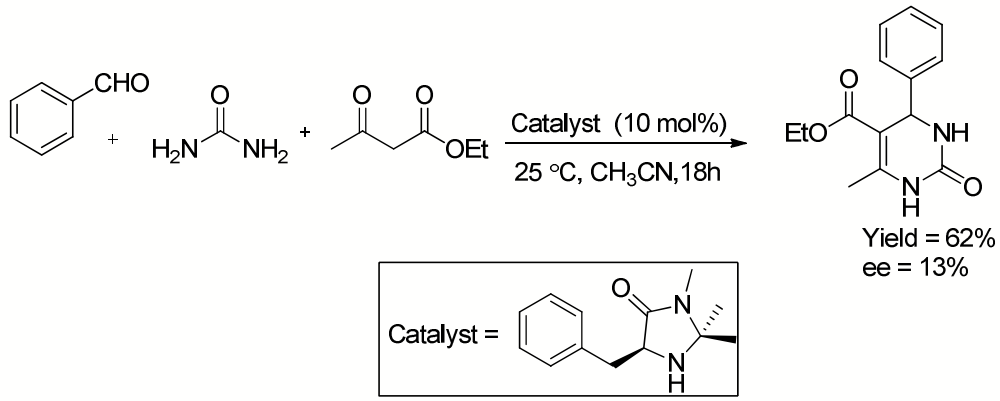
Abstract: Biginelli reaction is the multi-component reaction of aryl aldehyde, urea and ethyl acetoacetate to form 3,4-dihydropyrimidinones (DHPM). Dihydropyrimidinones (DHPMs) derivatives have exhibited important pharmacological properties like antiviral, antimalarial, antitumor, antihypertensive, antibacterial, analgesic, *anti*-inflammatory.[1-3]In our on-going efforts for development of modified MacMillan catalystfor asymmetric Diels-Alder reaction.[4] Herein, we have used MacMillan catalysts as Organocatalysts for asymmetric Biginelli reaction between benzaldehyde, urea and ethyl acetoacetate in acetonitrile at room temperature and corresponding 3,4-dihydropyrimidinone was afforded in 62% yield and 13% *ee* after 18 hours.



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P-44

"Stereoselective Synthesis of Deoxyglycosides and Glycomimetics From Glycals"

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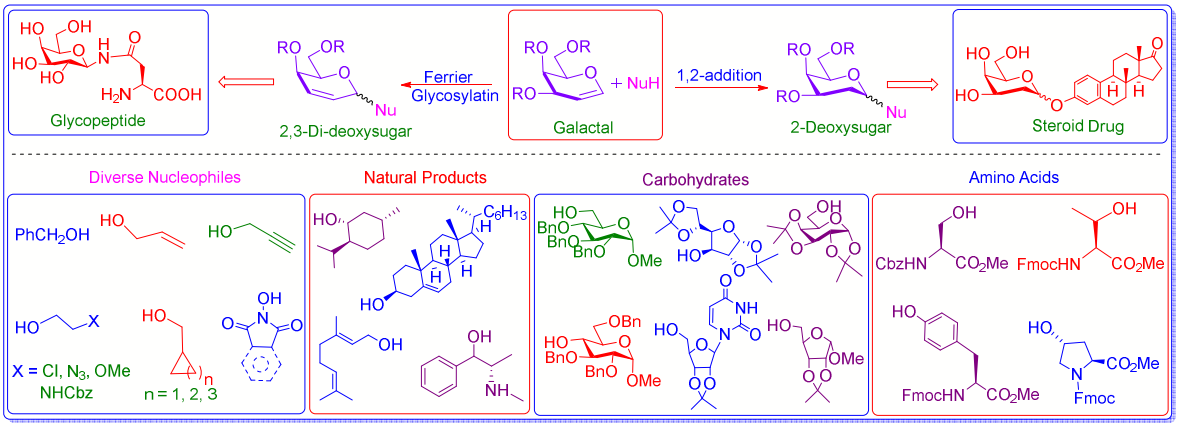
Abstract :The stereoselective synthesis of 2-Deoxy and 2,3-di deoxysugarsare particularly important due to their usefulness askey intermediates in the synthesis of several biologically important molecules,[1] such as antibiotics,[2]oligosaccharides,[3] carbohydrate derivatives.Deoxyglycoside are often found as components of a widerange of natural products having biological activity. [4-6]
As a part of our ongoing research towards the synthesis of glycosides and glyco-conjugates,[7]we explore the possibility of using Lewis acid catalyst for stereoselective synthesis of deoxyglycosides with variety of *O*-nucleophiles.The current protocol involves stereoselective synthesis of gycoside with a variety of *O*-nucleophiles in presence of other sensitive groups. Scope of this method has been demonstrated for the nucleophiles comprising allylic, propargylic, natural products, carbohydrates, amino acids.



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P-45

MacMillan Catalyst Supported on Magnetic Nanoparticle as Recoverable Catalystfor Asymmetric DielsAlder reaction

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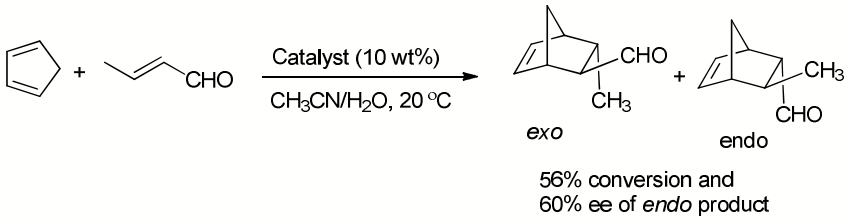
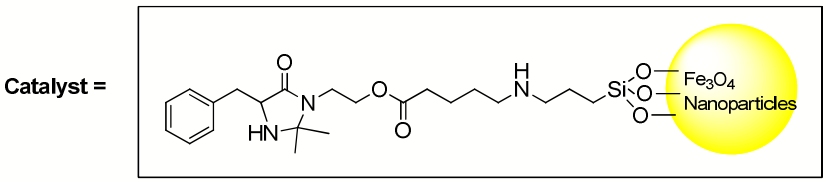
Abstract: Diels alder reaction is useful for the synthesis of 6 membered rings by [4+2] cycloadditionreaction between a conjugated alkene or substituted alkene. Diels-Alder reaction between cyclopentadiene and α-β unsaturated aldehyde (crotonaldehyde) to synthesize endo/exo-bicyclo[2,2,1]-hept-5ene carbaldehyde.[1-3]We have modified theMacMillan catalyst with magnetic nanoparticles by ester linkage and act as recoverable catalyst for asymmetric Diels Alder reaction. The Diels Alder reaction ofcyclopentadiene and crotonaldehydein the presence of modified Macmillan catalysts (10 wt%) by using trifluoroacetic acid (5 mol%) as co-catalyst in acetonitrile-water (95:5) at 20°C, gave the product in 56% conversion and 60% *ee*.





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P-46

BinolTi Complexes as a Catalyst for the Asymmetric Ring Opening of Epoxide

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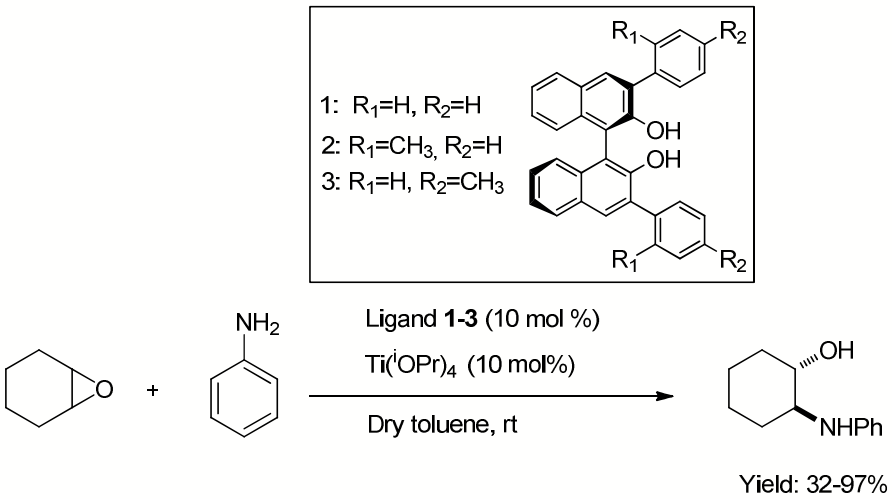
Abstract: Ring Opening of epoxide is the important transformation for synthesis of β-Amino alcohols. These are useful synthetic intermediates in the synthesis of a wide range of biologically active natural and synthetic products, chiral auxiliaries, unnatural β-amino acids, β-blockers in pharmaceuticals, and insecticides.[1]We have synthesized different derivatives of *R*-binol[2] such as (*R)*-3,3'-diphenyl-[1,1'-binaphthalene]-2,2'-diol, (*R)*-3,3'-di-o-tolyl-[1,1'-binaphthalene]-2,2'-diol and (*R)*-3,3'-di-p-tolyl-[1,1'-binaphthalene]-2,2'-diol. Here, we used these (*R*)-binol derivatives as a ligand in the ring opening of cyclohexene oxide with aniline in the presence of metal.[3]



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P-47

Exploration of Marine Sources for Microbial Beta Secretase Activity in the Management of Alzheimer's disease

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Abstract: Alzheimer's disease (AD) is a progressive neurodegenerative disease and is the major cause of dementia in the elderly. The complications in AD, leading to severe form of dementia associated with loss of memory is due to formation of amyloid plaques, hence the strategy for effective clinical management of AD should include the prevention of deposition of amyloid. Inhibition of Beta secretase enzyme can reduce the amyloid plaque deposition, which can stall the progression of the disease [1]. Marine microbes represent an indispensable source for therapeutically important bioactive molecules and are the most underexploited natural resources [2]. Few research studies have shown that the marine microbes such as algae, bacteria and fungi are capable of inhibiting the key enzyme involved in the pathogenesis of Alzheimer's disease such as beta secretase [3]. Microbes were isolated using selective marine agar and potato dextrose media from the deep sea sediments collected away from coast of Surathkal, Karnataka.The isolates were grown in a suitable production medium andsubjected to extraction using ethyl acetate (1:1 ratio). The ethyl acetate fractions of the isolates were screened for Beta secretase inhibitory activity. A total of 25 bacterial isolates were selected from the marine sediments.Out of the 25 bacterial isolates, crude ethyl acetate extractof "4FSS4" showed the highest inhibition Beta secretase inhibition (53.97%). The standard inhibitor (LY2886721) showed 79.28% inhibition. The active isolate was found to be *Aspergilllusiranicus*through 16s rRNAsequencing. Beta secretase inhibitors from marine microbes can be a novel therapeutic candidate in AD management.

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P-48

Anti-atrophic potential of CNA: Suppression of altered ROS, cytokines, and proteolytic systems by CNA in TNF -treated myotubes

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Abstract: Skeletal muscle atrophy under diverse conditions *i.e.* increased physical inactivity, aging and clinical settings *i.e.* cancer, diabetes, is silently posing a threat to human life due to non-availability of specified drugs. TNF□, a key mediator under such conditions/settings, is attributed not only inflammatory property but also oxidative stress which further exacerbates the inflammation and its associated consequences. Cinnamaldehyde (CNA), an active constituent of *Cinnamomum sp*, possesses diverse pharmacological activities including anti-diabetic, anti-cancer *etc* due to its regulatory effect on pro-inflammatory cytokines secretion and oxidative stress. Considering impact on inflammation and oxidative stress, we explored the potential of CNA against TNF□-induced myotube atrophy. C2C12 myotubes were treated with TNF□ (25ng/ml) in the presence or absence of CNA (50µM). The myotube morphology (*i.e.* length and diameter) was protected from atrophic effect of TNF□ upon 4h pre-incubation with CNA. The level of p65 and its mediated endogenous cytokines (TWEAK, IL1□) were observed low as were the level of reactive oxygen species in TNF□-treated cells incubated with CNA. Elevation in the level of lipid peroxidation and its mediated membrane injury was also inhibited by CNA in TNF□ exposed cells. Further, CNA moderates the degradation of muscle-specific protein (*i.e.* MHCf) by preventing the up-regulation of proteolytic systems (*i.e.* MuRF1/Atrogin1) and down-regulation of protein anabolic targets (*i.e.* Akt/mTOR) in the TNF□-treated myotubes. Our findings demonstrate that by preventing the production of reactive species and inflammatory cytokines and also by maintaining the protein metabolism homeostasis, CNA protects myotubes from TNF□-induced atrophy.

Keywords: TNFα, CNA, oxidative stress, NFκB, myotubes, atrophy

P-49

Synthesis of Sugar Chalcone Conjugates through Click Chemistry and Evaluation of their Biological Activity

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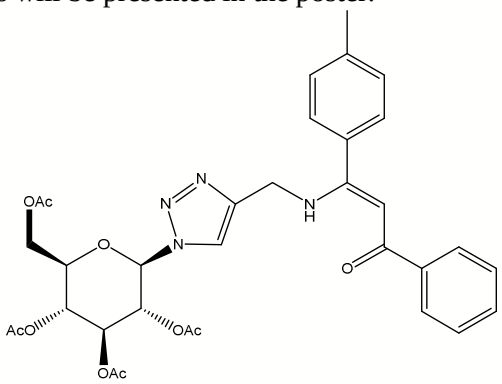
Abstract: Click chemistry has evolved as an important synthetic tool to synthesize diverse products of chemical and biological significance. Mimics of natural products and conjugate of biologically important molecules such as conjugate of sugar chalcone, sugar quinone, sugar coumarin, sugar lipids and sugar peptide are few examples of biologically significant sugar conjugates.

In the present work, we report the synthesis of 4-[*Z*-3'-(methylamino)-1'-phenyl-3'(p-tolyl)-prop-2'-en-1'-one]-1-(2'',3'',4'',6''-tetra-*O*-acetyl- -D-glucopyranosyl)-1,2,3-triazole and related analogues through conjugation of (2R,3R,4S,5R,6R)-2-(acetoxymethyl)-6-azidotetrahydro-2H-pyran-3,4,5-triyl triacetate with (Z)-1-phenyl-3-(prop-2-yn-1-ylamino)-3-(p-tolyl)prop-2-en-1-one in good to high yields. Details of the synthesis will be presented in the poster.



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P-50

Design, Multicomponent Synthesis and Characterization of Diversely Substituted Pyrazolo[1,5-a] Pyrimidine Derivatives

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Abstract: The synthesis of various heterocyclic compounds using acetoacetanilide[AAA], we have demonstrated that acetoactanilide are versatile intermediate for the synthesis of pyrazolopyrimidine derivatives. Thus, to explore further, we sought that the reaction of various acetoactanilide, an appropriate aldehyde and 5-amino-N-cyclohexyl-3-(methylthio)-1H-pyrazole-4-carboxamide in the presence of base in isopropyl alcohol could be an effective strategy to furnish the novel pyrazolopyrimidine derivatives. Here we describe the novel synthetic methodology for the fused pyrazolopyrimidines.

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synthesis, crystal structures and biological activity of some pyrazole and 1, 2, 3-triazole containing heterocyclic compounds

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Abstract: As heterocyclic compounds shows good biological activity so we synthesize nitrogen containing compound assuming that it gives some good results. N'-((5-chloro-3-methyl-1-phenyl-1H-pyrazol-4-yl)methylene)-5-methyl-1-phenyl-1H-1,2,3-triazole-4-carbohydrazide was synthesized from 5-(aryloxy)-3-methyl-1-phenyl-1H-pyrazole-4-carbaldehydecarbaldehyde and 5-methyl-1-(Halophenyl)-1H-1,2,3-triazole-4-carbohydrazide by condensation in acidic media. 5-(aryloxy)-3-methyl-1-phenyl-1H-pyrazole-4-carbaldehydecarbaldehyde and 5-methyl-1-(Halophenyl)-1H-1,2,3-triazole-4-carbohydrazide were synthesized from phenyl hydrazine and substituted anilines respectively. All intermediates and final compounds were confirmed by ^{1}H NMR, ^{13}C NMR and IR Spectroscopy methods.

P-52

Efficient synthesis of (*E*)-1-aryl-3-(glucal-1-yl)-propinones

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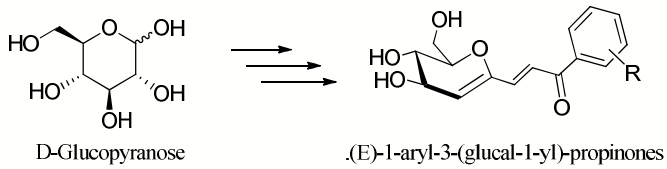
Abstract: Development of efficient synthesis of biologically active carbohydrate derivatives has drawn attention of glyco-chemists and glyco-biologists. Unsaturated sugar derivatives have shown anti-HIV, anti-influenza and many other biological properties, and have served as precursor for the synthesis of vineomycin B_2 antibiotics. Synthesis of C2 substituted unsaturated sugars have been reported by Heck coupling and Wittig reaction, whereas the synthesis of C1 substituted unsaturated sugars rely on C1 metalated glycals, C1 haloglycals and C1 glycal phosphates. Introduction of an α,β-unsaturated carbonyl system at C1 or C2 position of unsaturated sugars provided opportunity for synthetic elaboration of the carbon skeleton, which can lead to a variety of natural and unnatural *C*-glycosides for varied applications.

Herein, we have developed an efficient, convenient and one step method for the synthesis of C1 functionalized unsaturated sugar derivatives, *i.e.* (*E*)-1-aryl-3-(glucal-1-yl)-propinones from 2,3,4,6-tetra-*O*-benzyl-1-formyl-*β*-D-glucopyranose by condensation with aryl methyl ketones.



D-Glucopyranose .(E)-1-aryl-3-(glucal-1-yl)-propinones

Compds.	**a**	**b**	**c**	**d**	**e**	**f**	**g**	**h**	**i**	**j**
R	H	4-Me	4-OMe	2-OH	4-Cl	4-Br	4-NO_2	3-Br	3,4-O-CH_2-O-	4-OH

Acknowledgements: We are thankful to the University of Delhi for providing financial support under DU-DST Purse Grant & Scheme to Strengthen Research and Development, and to CIF-USIC of the University for providing Mass and NMR recording facility. BS is thankful to Deshbandhu College, University of Delhi, Delhi for providing suitable leave to Pursue PhD under career development program.

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P-53

Regioselective Rh(III) Catalyzed C-H Alkylation and Annulation with β-CF_3-Substituted Enones

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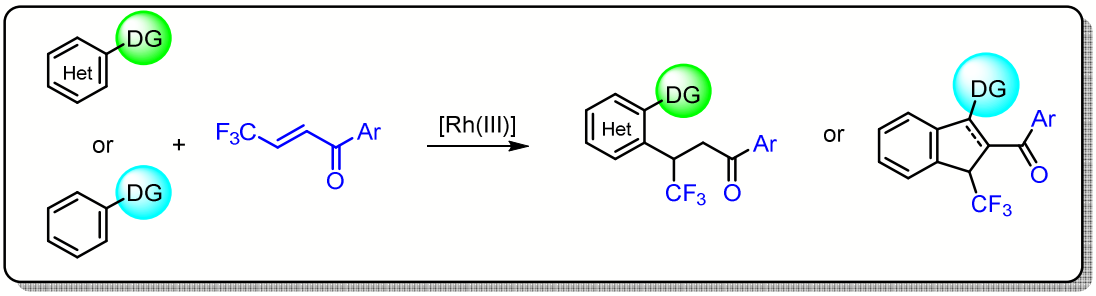
Abstract: The trifluoromethyl (CF_3) group is found in many biologically active molecules of pharmaceuticals and agrochemicals. In particular, incorporation of CF_3 group has been proven to increase lipophilicity, solubility, metabolic stability and bioavailability of many bioactive compounds. [1] Numerous methods have been developed for the installation of the CF_3 group into a variety of organic molecular structures. [2] However, alternative pathways for synthesizing molecules containing CF_3 moiety are always required in modern organic synthesis. In this context CF_3 containing building blocks plays an important role. [3] In addition, transition metal catalyzed C-H functionalization has witnessed major advances in the recent years.[4] Among them, C-H activation with olefins has made a huge impact in the field of organic chemistry and provides an easy access to various olefinated, alkylated and heterocyclic compounds

.

Reports of conjugate additions for β-trifluoromethyl-α,β-unsaturated ketones are scarcely reported via directing group assisted C-H activation. [5] To this end, herein we report an efficient strategy for the synthesis of diverse molecules containing trifluoromethyl group under Rhodium (III) catalysis.



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P-54

A one-pot multicomponent synthesis of 2-amino-4*H*-chromenes: An efficient green approach using triethanolamine as catalyst in aqueous medium

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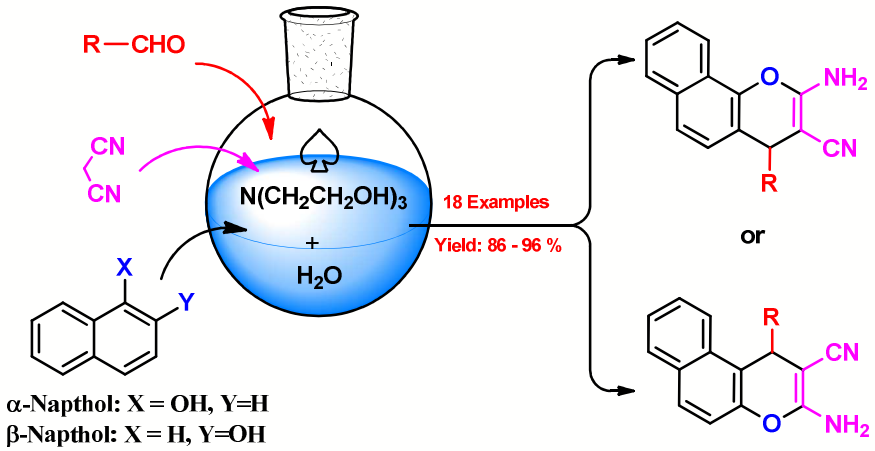
Abstract: An improved simple and facile synthesis of 2-amino-4*H*-chromenes by employing three component one-pot condensation reaction of heterocyclic/aromatic aldehyde, (□□□)-naphthol and malononitrile using triethanolamine in water. The advantages of this method are the use of triethanolamine, an inexpensive, ecofriendly and readily available catalyst, easy workup, excellent yields, and the use of water as a green solvent.

Keywords: 2-amino-4*H*-chromene, Triethanolamine (TEOA), multi-component reaction, aqueous media, green synthesis



P-55

C-5 Curcuminoids: Synthesis and antibacterial activity against Staphylococcus aureus and their mechanistic studies

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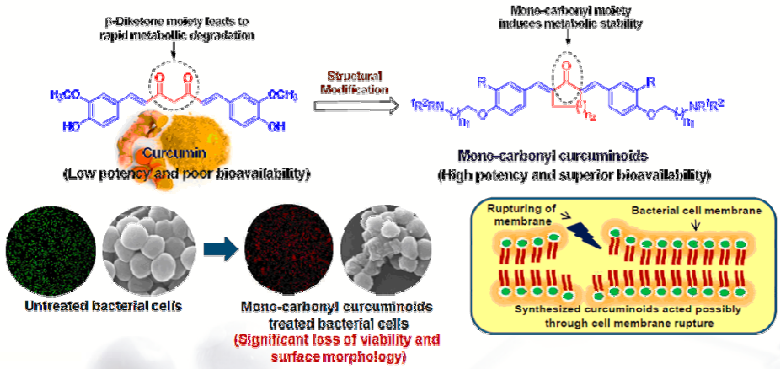
Abstract: Curcumin, a natural product isolated from the *Curcuma longa* L., rhizoma, has been known for its diverse pharmacological effects with no toxicity [1,2]. But its therapeutic potential is severely restricted because of its low aqueous solubility and poor stability under physiological conditions. In order to overcome these limitations, medicinal chemist has made several modifications, and one of the modification deals with the shortening of the central β-diketone from C7 to C5. This approach has resulted many compounds with better anticancer activity [3-5]. Encouraged by these studies, we modified the central β-diketone part of the molecules[6-9]. and attached various biocompatible groups in the aromatic portion of the molecule and studied their anti-bacterial activity against *S. aureus*. Out of the library of 50 compounds screened, twenty three compounds displayed potent antibacterial activity against clinically relevant *Staphylococcus aureus* with the IC_{50} value in the range of2 to 32 µg/mL.These curcuminoids were found to be very stable at physiological conditions and did not cause any toxicity towards mammalian cells. The best active curcuminoidscaused instant membrane depolarization and were able to permeabilize the bacterial membrane, which could be the reason for their potent bactericidal activity and some of them killed staphylococcus cells without damaging the bacterial membrane. Overall, the present work established the *Staphylocidal* potency of water-soluble, non-toxic curcuminoids thereby providing an impetus for the development of these leads for therapeutic use against *S. aurues*.



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P-56

'ONE-POT SEQUENTIAL APPROACH FOR THE CONSTRUCTION OF HIGHLY FUNCTIONALIZED TRIAZOLO[4,3-c]PYRIMIDINES'

Khushbu Dodeja, Yogesh Bhola, Mayur Shiyal Corresponding Author: Prof. Y. T. Naliapara*

Abstract: Novel1,2,4-triazolo[4,3-c]pyrimidine-8-es were synthesized via oxidative cyclization of hydrazono-1,6-dihydropyrimidine-5-e application of iodobenzenediacetateasasole cyclizing agent. Here, were port a one-pot sequential strategy to generate the corresponding triazolo pyrimidines by condensation of pre prepared acylketenedithioacetals and rylamidines. Moreover, this process describes the application of presynthesized arylamidines, which omits the Suzuki-Miyaur across-coupling reaction and hence provides metal-free organic synthesis in an atom and step economical fashion.

Keywords:
Metal-free orgenic synthesis, Iodobenzenediacetate as cyclizing agent, simple synthetic procedure with high yield.

P-57

Click Synthesis, Molecular Docking and Anticancer Evaluation of New Series of Saccharine-Triazole Hybrid Molecules

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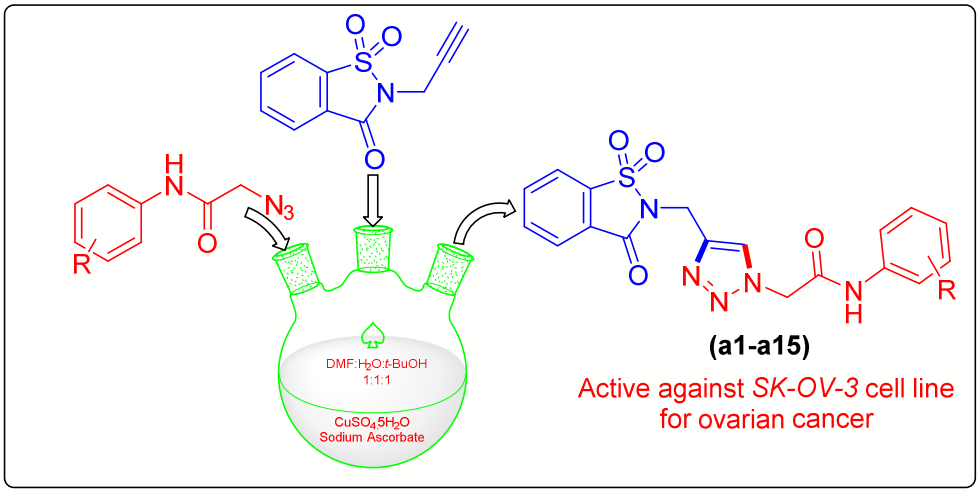
Abstract:



The design and synthesis of a new series of saccharine–triazole hybrids as potential anti-cancer agents is described. The new hybrid molecules were synthesized *via* copper(I) catalyzed [3+2] azide–alkyne cycloaddition and showed excellent binding affinity towards non-receptor tyrosine kinase inhibitorwhen subjected to virtual screening based on molecular docking. The molecular docking results were experimentally validated by 60 cell line study against cancer cell lines. The compounds show excellent activity against *SK-OV-3* Ovarian cancer cell line are promising for the development of potential anticancer drugs based on these new molecules

.

Keywords: Click chemistry, Molecular Docking, Saccharine-triazole hybrid, anticancer agents, ovarian cancer

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P-58

Novel CuO@NiO nanoparticles catalysed synthesis of biologically active Indenoisoquinoline derivatives.

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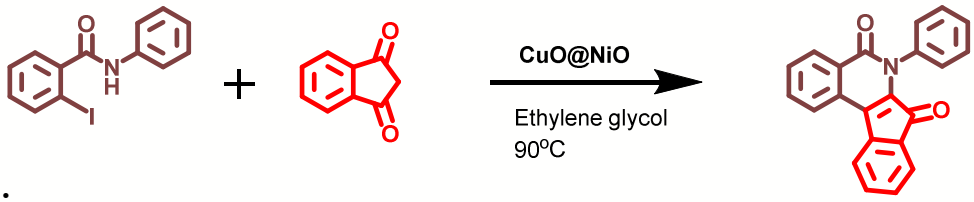
Abstract: denoisoquinolines are novel topoisomerase I inhibitors,[1] which act as anticancer agents[2] and found to be effective in treating visceral leishmaniasis.[3] Various methods have been reported for synthesis of Indenoisoquinolines involving multiple steps, complicated starting materials and restricted substrate scope.[4-6] To avoid these shortcoming and in continuation of our work towards synthesis of biologically active heterocycles using nanocatalyst,[7-10] a novel nanocatalyst CuO@NiO has been synthesized and characterized which can be used for synthesis of biologically active Indenoisoquinolines from 2-Iodobenzamide and 1,3-indanedione without using base and additives in recoverable solvent ethylene glycol. CuO@NiO nanocatalyst can be prepared by calcination of mixture of malachite as sustainable copper source and Nickel oxalate at 400℃ for 4h. CuO@NiO nanocatalyst was found to be better and robust catalyst as compared with CuO nanoparticles for synthesis of Indenoisoquinolines with better values of green chemistry metrices like low E factor, high reaction mass efficiency and high atom economy. Nanocatalyst can be recycled and reused upto five reaction cycles without major loss in its catalytical activity.



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P-59

Herbometallicnano-drug impairing mitochondrial metabolic alteration in breast cancer cells

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Abstract: Despite a remarkable improvement in the field of cancer diagnosis and chemotherapy, cancer still become a threat due to frequent cellular and molecular alteration along with the side effects of promising drugs and techniques day by day. Now a days, natural compound based drug therapy has been getting a great attention due to lower side effects and multiple effective target points against several cancer types. Here, we have reported the synthesis and characterization of a novel herbometallic compound having effective interference with mitochondrial metabolic alterations related cancer progression and programmed cell death in breasrt cancer cell lines. Biocompatibility of the compound was investigated through inductively coupled plasma optical emission spectrum (ICP-OES), Differential light scattering (DLS), field emission scanning electron microscopy (FESEM), cell cytotoxicity assay (MTT asssay)etc. Cellular metabolic alterationswere investigated through the measurement of cellular antioxidant level (GSH/NADPH), reactive oxygen species (ROS) and ATP productions along with induction of programmed cell death or cell apoptosis in breast cancer cell lines.

Keywords: herbometallic compound, inductively coupled plasma optical emission spectrum, cellular antioxidant, ROS, apoptosis

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P-60

SYNTHESIS, SPECTROSCOPIC, THERMAL AND FLUORESCENCE STUDIES OF SOME TRANSITION METAL BASED HETEROCHELATES

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Abstract: 4-acyl pyrazolone derivatives and their heterochelates are well known for their thermal and fluorescence activity. Modi et al.[1,2]. However, here we represent the fluorescence and thermal studies of some 4-acyl bis pyrazolone Schiff bases as ligand and their transition metal heterochelates. Structural and spectroscopic properties have been studied on the basis of elemental analysis, FT-IR, ^{1}H-NMRandfluorescence spectral studies. The structure of heterochelates confirmed by thermal analysis (TG/DTG curve) and FAB mass spectra. The ligands and their hetero chelates are studied at room temperature for their fluorescence study. It is observed from the data that the fluorescence spectra of heterochelates gives slight Bathochromic shift from the fluorescence spectra of ligands, which may be due to the chelation of ligands with the transition metal ions.

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P-61

An efficient copper-mediated aerobic oxidative synthesis of Benzimidazo fused quinazolines

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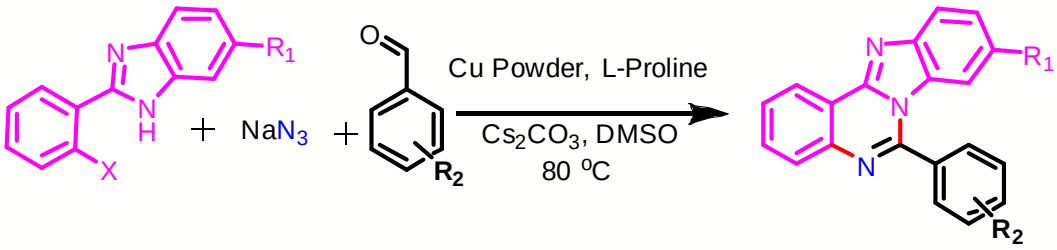
Abstract: Copper mediated aerobic oxidative multi-component synthesis of benzimidazo [1,2-c]quinazoline derivatives has been developed using sodium azide as nitrogen source from readily available 2-(2-halophenyl) benzoimidazoles and aldehydes. This protocol involves azidation of haloaryl with sodium azide followed by *insitu* conversion of azide into arylamine, which on condensation with benzaldehyde afforded benzimidazo [1,2-c]quinazoline in good yield.we have demonstrated first copper catalysed multicomponent synthesis of diverse benzimidazo[1,2-c]quinazolines in aerobic conditions from 2-(2-halophenyl benzoimidazoles, aldehyde, and sodium azide as nitrogen source. The reaction probably proceeds through in situ conversion of azide into arylamine flowed by condensation with aromatic aldehyde. We believe operational simplicity and economic of this procedure will find important applications in synthesis of nitrogen hetrocycles in the area of medicinal, and material chemistry



Scheme: Synthesis of Benzimidazo [1,2-c]quinazoline

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P-62

Design, Synthesis and Biological Activity of Novel *N*-Aryl-IndolesAs Potential Anti–Prostate Cancer Agents

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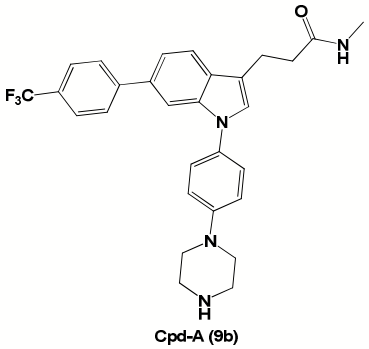
Abstract: Integrin-linked kinase (ILK) represents a promising therapeutic target for the prostate cancer.[1-3] In this study, we have design and synthesized several new *N*-aryl indole analogs for their anti-prostate cancer evaluation. Among the newly prepared derivatives, Cpd-A(**9b**) exhibited potent antiproliferative activity (IC_{50}= 2.3 □M) against the PC-3 cell growths in vitro. Moreover, western blot analysis revealed that **9b** inhibit ILK activity by consistent inhibition of the phosphorylation of AKT at Ser–473 and GSK3□□at Ser–9 in PC-3 cells. Having promising antiproliferative profile, compound **9b** can be considered as potential lead candidates for further development



Cpd-A (9b)

Design of N-aryl-indole derivative by scaffold replacement

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P-63

Copper-Catalyzed Decarboxylative Regioselective Synthesis of 1,5-Disubstituted 1,2,3-Triazoles

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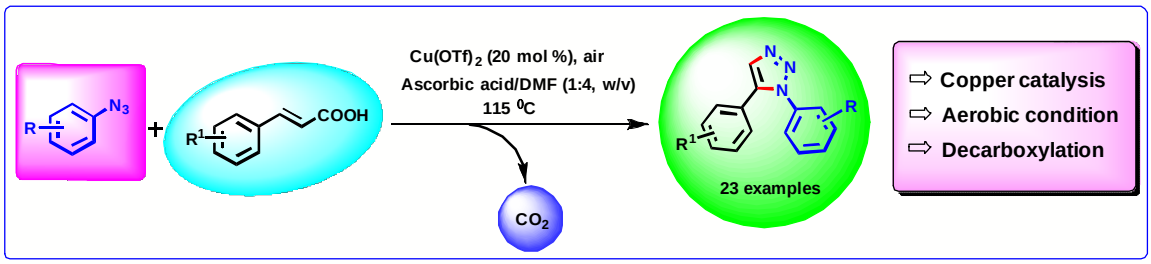
Abstract: A copper-catalyzed decarboxylative regioselective protocol for the synthesis of 1,5-disubstituted 1,2,3-triazoles through direct annulation of cinnamic acids with aryl azides has been developed. This is the first example of 1,5-disubstituted 1,2,3-triazoles, under aerobic condition using Cu (II) as the catalyst, which was generally synthesized by ruthenium (II) catalyst. The operational simplicity and regioselectivity of this methodology, complementing to the classical CuAAC catalyzed the synthesis of 1,4-disubstituted 1,2,3-triazoles.



Scheme: synthesis of the 1,5-disubstituted 1,2,3-triazoles

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P-64

Efficient and Rapid Synthesis of HighlyFunctionalized Novel Symmetric 1,4DihydropyridinesUsing Glacial AceticAcidas Solvent

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Email: rahulbhambhani6417@gmail.com

Keywords :1,4-Dihydro pyridines; glacial acetic acid; coumarino aldehyde

Abstract: A new series of 1,4-dihydropyridines bearing a coumarin moiety in the 3-positionwere synthesized by a variation of the classical Hantzsch synthesis. The reaction of derivatives of coumarin-3-aldehyde with 3-amino crotononitrile in the presenceof glacial acetic acid afforded novel 1,4-dihydropyridines.The procedure has short reaction time (15–20 min), easy workup, and good yield ofproduct. The structures of all synthesized compounds were well characterized by mass,infrared,^{1}H and^{13}C NMR.

P-65

Quantification of Sinapic Acid in Camelina sativa L. Defatted Seed Cake Using High Performance Thin Layer Chromatography

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Abstract: A simple, rapid and accurate method of High performance thin layer chromatography was developed for the validation and quantification of Sinapic acid in methanolic extract of Camelina defatted seed cake. There are various HPLC methods have been reported previously for the identification and quantification of sinapic acid in different extracts, but HPTLC provides an ideal confirmatory method which is cost effective and environmentally friendly as compared to HPLC. Methanolic extract of defatted cake was prepared using Soxhlet method. Analyses and quantification of sinapic acid was performed in precoated aluminium sheet TLC plate (Merck, Silica gel F254) as stationary phase. Samples were sprayed onto TLC plate in the form of bands with Nitrogen (Linomat 5) at the speed of 150 nl/sec. Development of Chromatogram was carried out in twin through glass chamber saturated with the standardized mobile solvent i.e. Ethyl acetate: Ethyl methyl ketone: Formic acid: water (5:3:3:1 v/v/v/v) at room temperature (25˚C ± 2). Densitometric evaluation (TLC Scanner 4) of developed chromatogram was done at 254 -336 nm (U-V range) using Deuterium and Tungsten lamp after spraying the developed plate with the Alcoholic Ferric chloride. System identified a clear spot of Sinapic acid at the R_f value of 0.936 (± 0.02). Linear graph shows the correlation coefficient (R) was 99.9952 %. The result observed clearly showed the intense band of sinapic acid with the value of 250.4 µg/mg. Statistical analysis of the data showed that the method is reproducible and selective for estimation of sinapic acid and its derivatives.

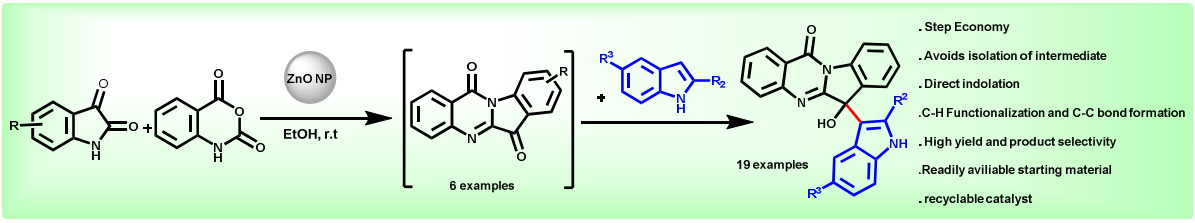
Keywords: Camelina defatted seed, HPTLC, Sinapic acid, Chromatogram, Mobile solvents

P-66

Zinc Oxide-NP Catalyzed Direct Indolation of *insitu* generated Bioactive Tryptanthrin

Ratnakar Dutt Shukla,[a,b] Byanju Rai[a] and Atul Kumar[*ab]

Abstract: A ZnO-NP catalyzed direct indolation of *insitu* generated tryptanthrin*via* C-H functionalization and C-C bond formation has been developed. This novel and greener approach has been effectively utilized to accomplish the synthesis of 6-hydroxy-6-(1*H*-indol-3-yl)indolo[2,1-*b*]quinazolin-12(6*H*)-one derivatives in good to excellent yield with highproduct selectivity. Besides *insitu* approach adirect indolation of tryptanthrin has also been developed.



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P-67

Synthesis of pyrano sugar-amino acidbasedmacrocycles for anion inclusion applications

Sandeep Kumar, Ankita Singh, Kavita and Ashok K. Prasad*

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Abstract: In the area of supramolecular chemistry anion complexation chemistry, specially carboxylate anion complexation is currently receiving much attention due to their chemical as well as biological roles, such as regulation of sulphate and phosphate anion in cell membrane, carrier of genetic information (DNA/RNA), enzyme-substrate interactions,carboxylate anion incarboxypeptidaseA, carboxylate anion in biological activity of vancomycin family of antibiotics etc.We have synthesizedmacrocyclic compounds using 2,6-anhydro-glucoheptitol, glycineand dicarboxylic acid linkers, *viz.* succinic acid and pyridine dicarboxylic acid. The anion inclusion capabilities of synthesizedmacrocyclic compounds have been evaluated using boc-GlyCOO$^-$anion*via* ^{1}H NMR titration studies in $CDCl_3$. The macrocyclic compound **1** and **III** have shown strong binding affinity towards carboxylate anion present in TBA salt of *N*-boc-glycine. The detailed synthetic protocol and binding data will be discussed during poster presentation.

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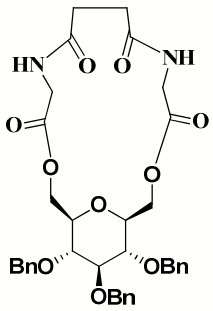
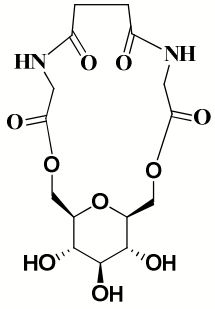
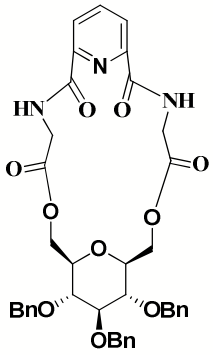


Macrocycle I



Macrocycle II



Macrocycle III

Acknowledgement- We are thankful to University of Delhi for providing financial support under DU-DST Purse Grant & Scheme to Strengthen Research and Development, and to CIF-USIC of the University for providing Mass and NMR recording facility. SK thanks CSIR (New Delhi) and AS thanks CFEES-DRDO Delhi for the award of Research Fellowships.

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P-68

CNA and its derivatives: Antioxidant properties and Potential protective agents against oxidative stress induced atrophy

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Abstract: Skeletal muscle atrophy is a consequence of many physiological and pathophysiological conditions and is often associated with increased morbidity, mortality and poor quality of life. Oxidative stress as an important mediator of atrophy, therefore, supplementation of antioxidant with multi-targeted approach may provide a new positive outlook. The present study reveals the structure activity relationship of synthesized derivatives of CNA in respect to observed effects and their efficacy as antioxidant agent and protecting agent against oxidative stress induced atrophy in C2C12 myotubes. MeCNA, BeCNA, HCNA, BrCNA and FoCNA compounds were synthesized and analysed. Determination of anti-oxidative potential using well defined DPPH, ABTS, Phosphomolybdate and Ferric chloride assay reveals that HCNA, CNA, MeCNA and BeCNA worked as better antioxidant than BrCNAs and FoCNA. However, at acidic pH MeCNA and FoCNA showed the maximum activity. The anti-atrophic effect of these derivatives in H_2O_2 induced atrophy in C2C12 myotubes was different than the invitro antioxidative potential observed. In C2C12 myoblast culture HCNA shows the most toxic effect as it culminate the proliferation and cell viability whereas CNA, MeCNA and BeCNA maintained normal morphology as examined by immunofluorescence, and bright-field microscopic examination indicating that it is not always obvious that good antioxidant is better drug for all cells. CNA, BeCNA and MeCNA showed pronounced protective effect in H_2O_2 induced atrophied myotubes. BeCNA and MeCNA showed quite good efficacy in their antioxidant and radical scavenging abilities, as well as anti-atrophic effect on C2C12 myotubes suggesting their therapeutic use in atrophy associated with stress conditions.

Key words: C2C12, CNA, CNA-derivatives, atrophy

P-69

Microwave-Assisted Rapid Synthesis of Novel1,5-Benzodiazepine Derivatives as Potent Antimicrobial Agent

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Keyword : Antimicrobial Agent, 1,5-Benzodiazepine

Abstract: A new series of highly functionalized 1,5-benzodiazepine derivatives have been synthesized from 3-[(1E)-N-(2-aminophenyl) ethanimidoyl]-4-hydroxyl-2H-chromen-2-one and pyrazole aldehyde using catalytic amount of triflouro acetic acid under microwave irradiation. The main significant of the present procedure is shorter reaction time, easy work up procedure, and excellent yield with high purity. The structures of all the compounds were established on the basis of their IR, NMR, and mass spectral data and have been screened for their antimicrobial activity and antifungal activity.

P-70

Mycobacterium tuberculosis membrane inhibitors: Design, synthesis, biological evaluation and ADME analysis

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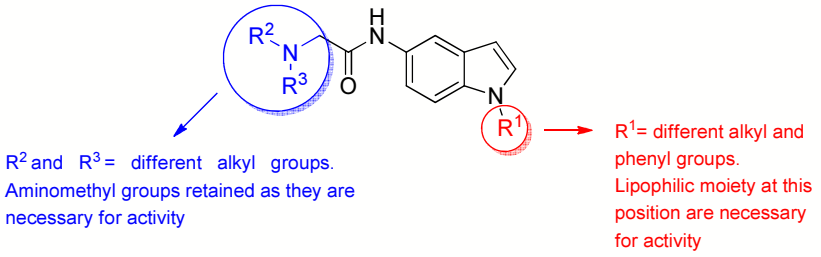
Abstract: *M. tuberculosis* membrane inhibitors have recently received much attention as anti-Tb drug target for its indispensable role in the survival of both replicating and dormant bacteria. Antimicrobials disrupt mycobacterial membrane either by interfering with the organization of lipid bilayer or by targeting the membrane-associated enzymes. Agents that disrupt the organization of the bacterial membrane are positively charged lipophilic molecules. Lipophilicity allows interaction with the lipid rich matrix of the outer membrane. The positively charged state allows accumulation in bacterial membrane which shows anionic behaviour because of the presence of phospholipids and polyanionic groups.[1]Indole based molecules are known for their wide range of biological activities and recently cationic amphiphilic indoles have been reported as antimycobacterial agents.[2] In continuation to our studies towards the development of anti-TB agents, [3-6] we designed cationic amphiphilic indole derivatives with an aim to improve the therapeutic potential of the resulting molecules. The side chain at indole nitrogen (R^1) adds to the lipophilicity of the compound while the secondary amines contribute to cationic state of compound. These analogs were then evaluated against *M. tuberculosis.* These cationic amphiphilic molecules hold the potential for better mycobacterial membrane inhibitors.



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P-71

Regioselective Synthesis of Fused Imidazo[1,2 a]pyrimidines viaIntramolecular C−N Bond Formation/6-Endo-Dig Cycloisomerization

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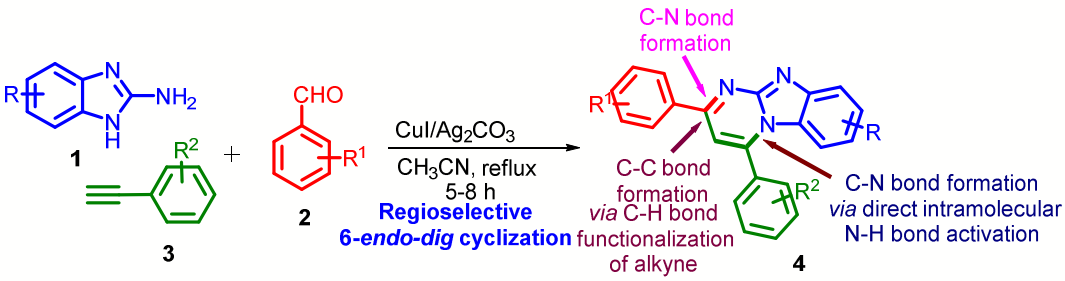
Abstract: An efficient regioselective cascade synthesis ofN-fused imidazo heterocycles has been developed. Thiscascade transformation proceeds via a transition-metal(copper/silver) catalyzed coupling reaction between 2-aminobenzimidazole,aldehydes, and alkynes leading to the formationof propargylamine intermediate, which regioselectively undergoes6-endo-dig cyclization through intramolecular N−H bondactivation interceded C−N bond formation leading to highly functionalized imidazo[1,2-a]pyrimidines in good toexcellentyields.



Scheme: Synthesis of diaryl-pyridinium-azaarenebutenolatezwitterionic derivatives.

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P-72

Phytochemical study of CapparisZeylanicaLinn. roots extract

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Abstract: In this study, we isolated, identified and characterized the phytoconstituents of *CapparisZeylanica*Linn. alcoholic root extract. The extract was analyzed by GC-MS between 0 to 30 min time intervals. The extract was further eluted in column using petroleum-ether - chloroform and chloroform - ethanol at different combinations. Identity of the constituents isolated was confirmed by comparing data of physicochemical and spectral characteristics (M.P., UV, IR, Mass, 1H and 13C NMR spectra) with the reported data in literature. Five compounds were obtained by column chromatography of the extract are β-amyrin, stachydrine, stigmasterol, decanoic acid (Capric acid) and 4-hydroxy benzoic acid. GC-MS study also revealed several biologically active compounds. Based on the results obtained, it is possible to conclude that ethanolic extract of *Cappariszeylanica*roots have biologically active compounds which would be responsible for the biological activity.

Key words: Triterpenoid; Stachydrine; *CapparisZeylanica*; n-Decanoic acid.

P-73

RGO@CuI composites and Ni@CuI core-shellsas recyclable nanocatalysts for the synthesis of biologically active N-heterocycles

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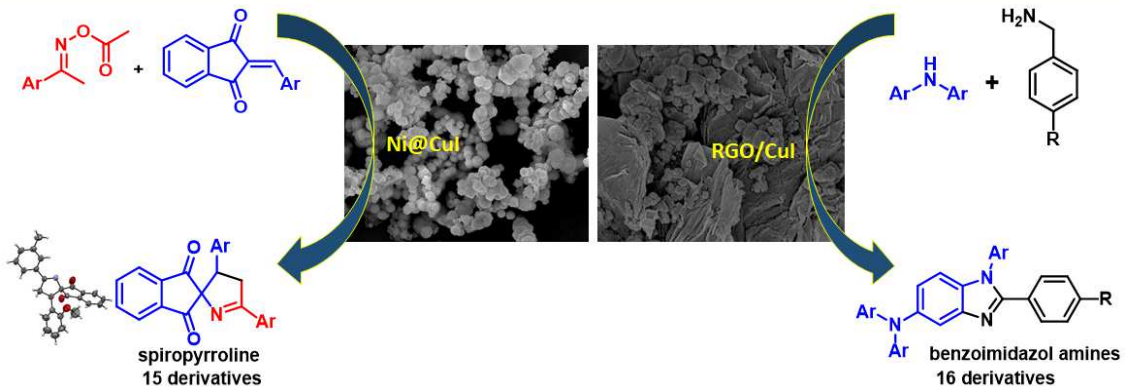
Abstract: Development of recyclablenanocatalysts for the construction of value-added synthons and bioactive heterocycles from renewable feedstock derived commodity chemicals is a great interest of sustainable chemistry.[1]With this inspiration, our group has been focused on designing nanocatalysts for A3 coupling strategies and decarboxylative C(sp^3)-H activation of feedstock derived substrates such as amino acids, aromatic aldehydes and amines.[2-10]The present study focused on design of CuI based nanocatalysts such as RGO@CuI composites and Ni@CuI core-shells for improved synthesis of benzoimidazol amine and spiropyrroline N-heterocycles. These skeletons are abundant core of natural products with several biological activities such as antiviral, antimicrobial andalleviation of neuropathic pain.RGO@CuI and Ni@CuI nanocatalysts were robust and recyclable up to six times with wide substrate scope and good functional group compatibility, high yields and short reaction time. The present approach showed ideal green chemistry metrics with low E-factor, high atom-economy and high turnover number which makes this process green and sustainable.



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P-74

One-Pot Preparation of Highly Substituted Pyrimidine Derivatives Using Amidine and Ketene dithioacetals.

Vidya V. Jadvani, Bhoomi M. Makwana, Y.T.Naliapara*

(Department of Chemistry, Saurashtra University, Rajkot-360005, Gujarat, India).

Abstract: A simple, convenient and efficient one pot synthesis of fully substituted pyrimidines was developed by cyclocondensation of α- oxo ketene dithioacetals with amidine in the presence of potassium carbonate in good yield. Structures of all the newly synthesized compounds were elucidated by elemental analysis and spectral analysis.

P-75

Synthesis of Double-headed Nucleosides from D-Glucose

Vineet Verma and Ashok K. Prasad*

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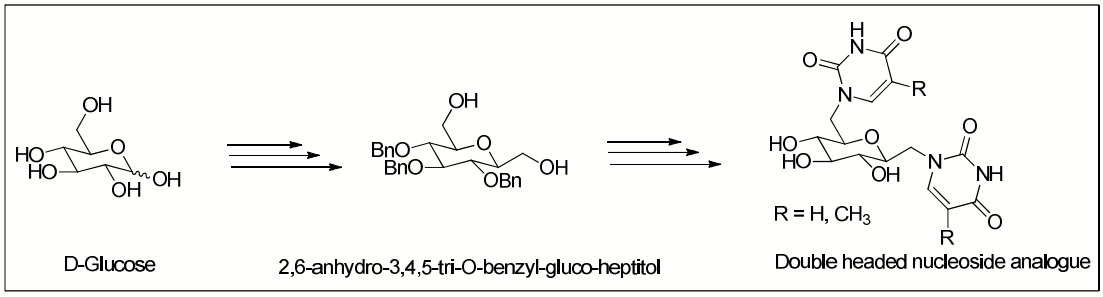
Abstract: Nucleoside and their analogues can be used as therapeutic agents for the treatment of several diseases, such as antiviral, antibacterial, anticancer, etc. They can also be used as potent glycosidase inhibitors. Some research groups have synthesized double-headed nucleosides which can be incorporated in DNA duplex to establish various intra or extra helical contacts depending on the location of second nucleobase which provides extra stability to the duplex.
Herein, we report the synthesis of novel double headed nucleoside analogues starting from D-Glucose. The synthesis of dihydroxy precursor, 2,6-anhydro-3,4,5-tri-*O*-benzyl-glucoheptitol was carried out starting from D-glucose which was further converted into ditosylated sugar. This ditosylated sugar derivative was then converted into double headed nucleoside derivative. These novel compounds will be evaluated for their biological activities.



Acknowledgement- We are thankful to the University of Delhi for providing financial support under DU-DST Purse Grant & Scheme to Strengthen Research and Development, and to CIF-USIC of the University for providing Mass and NMR recording facility. V.V. thanks CSIR for the award of Junior Research Fellowship.

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P-76

Convenient Route for the Synthesis of Substituted Chromanes from D-Mannose

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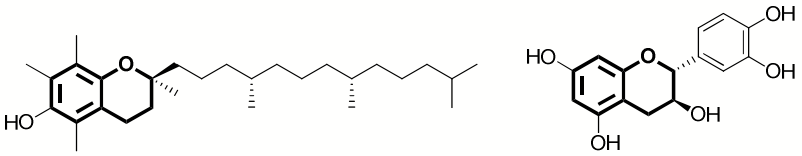
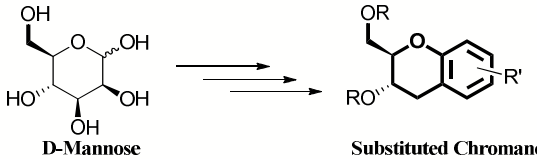
ashokenzyme@gmail.com

Abstract: Chromanes are associated with a broad range of biological and pharmaceutical activities such as antioxidant, anticancer, antidiabetic, antihypertensive, etc. Due to the biological importance of chromanes, efforts have been made to develop an efficient and selective synthetic method to afford these molecules.



α- Tocopherol (+)- Catechin

Most of the known methods in literature use pertinently functionalized aromatic moiety as starting compound in order to annulate the pyran system. Fusion of an aromatic system with pyranosugar to synthesize chromanes is still an arduous task in synthetic organic chemistry. We have developed a new strategy for the formation of chromane core using metal catalyzed oxidative C-H activation followed by subsequent cyclization / dehydrogenation from *C*-1substituted glucal which is derived from mannose.



D-Mannose Substituted Chromanes

Acknowledgement- We are thankful to the University of Delhi for providing financial support under DU-DST Purse Grant & Scheme to Strengthen Research and Development, and to CIF-USIC of the University for providing crystallographic data and NMR recording facility. VKM thanks CFEES-DRDO Delhi for the award of Junior Research Fellowship.

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P-77

TBHP-Promoted Oxidative Ring Opening of Unprotected 2-Aryl/Alkylindoles: A Simple and Efficient Synthesis of 2-Amidobenzoic Acid Derivatives under Metal-free Conditions

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Abstract: 2-Amidobenzoic acids derivatives are most common structural cores present in a variety of bioactive compounds and natural products. These structural motifs are reported to exhibit various biological activities namely antimicrobial (PqsD inhibitors), RNA polymerase inhibitors, plasminogen activator inhibitor-1 (PAI-1) and Pax-2- inhibitors.[1] In addition, these compounds are also primary building blocks in organic synthesis and medicinal chemistry. Owing to their valuable synthetic and biological applications, development of new and efficient synthetic methods to synthesize of amidobezoic acid molecules would be an active research in organic synthesis. On the other hand, peroxides have received great attention in organic synthesis,[2] we herein, disclose a simple and highly efficient strategy for the synthesis of 2-amidobenzoic acid derivatives from 2-ary/alkyllindoles *via* oxidative cleavage under metal-free and base free conditions. The reaction tolerates a wide range of functional groups and allows an assembly of medicinally applicable 2-amidobenzoic acid derivatives in good to high yields. Radical trapping experiments revealed that the present metal-free transformation involved a radical pathway. Practical application of the method was justified with gram scale reaction.

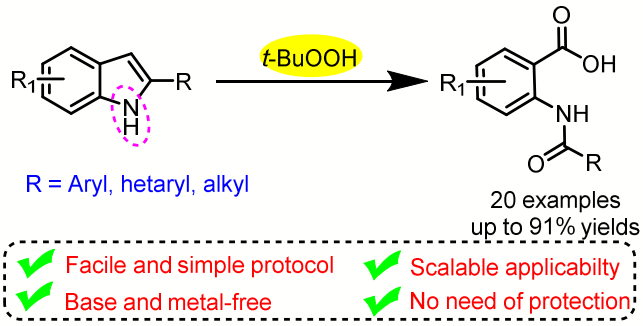

Figure 1. Synthesis of amidobenzoic acids

References:

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P-78

Design and Synthesis of Imidazo/Benzimidazo[1,2-*c*]quinazoline Derivatives and Evaluation of their Antimicrobial Activity

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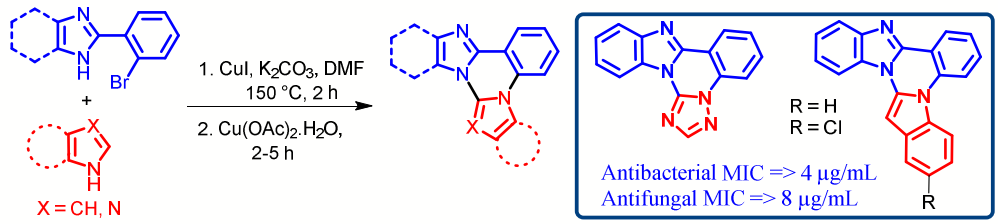
Abstract: Transition metal–catalysed cross coupling and C-H activation/ functionalization reactions have emerged as powerful tools for the construction of diverse array of useful heterocycles in medicinal chemistry and material science. In recent year remarkable progress has been made for the construction of functionalized heterocycles *via* copper catalysed tandem reactions. Construction of quinazolines, based π-conjugated system has recently been the subject of growing interest owing to their application in material science.[1] Additionally, molecules with these moieties have shown wide range of biological properties such as anticancer, antimalarial, analgesic, antiulcer, anticonvulsant, antitumor, diuretic and antihypertensive.[2] With the advent of interest in π-expanded heterocyclic compounds.[3] we developed an efficient and convenient synthetic protocols for fused quinazolines (**Scheme 1**). A new class of fused quinazolines has been synthesized *via* a copper–catalysed Ullmann type C–N coupling followed by intramolecular cross-dehydrogenative coupling (CDC) reaction in moderate to good yields. The synthesized compounds were tested for *in vitro* antibacterial activity against three Gram negative and two Gram positive bacteria. The synthesized compounds were also evaluated for their *in vitro* antifungal activity against *Aspergillus niger* and *Candida albicans.* Moreover, the haemolytic activity of the synthesized compounds showed their safety profile towards the human blood cells



Scheme1. Synthesis of Imidazo/Benzimidazo[1,2-*c*]quinazoline derivatives

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P-79

Synthesis of Coumarin and Quinolinones Fused Aza-heterocycles *via*Ullmann Type C-N Coupling Reaction and Cross-dehydrogenative Coupling

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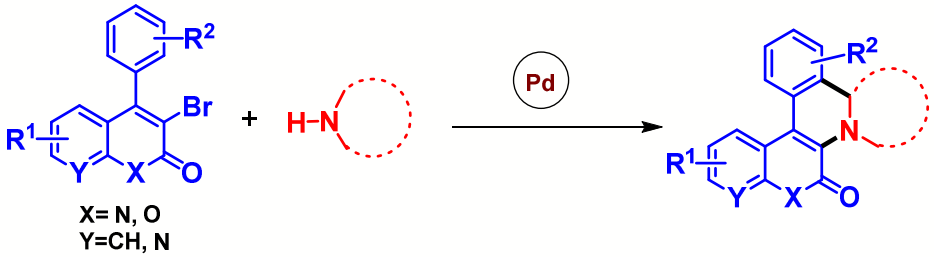
Abstract: Formation of targeted C-C bond is quite difficult task in chemistry because of unreactive starting material.Transition metal-catalyzed functionalization of unreactive C-H bonds has been successfully exploited for the formation of C-C / C-Heteroatom bonds due to its selectivity and atom economy feature, which makes this strategy more environment friendly as compared to traditional cross coupling reactions.[1]

Coumarin and quinolinonesare key motifs of many biologically active molecules such as Scoparone, Dicoumarol, Osthole.[2] Additionally, such compounds have a numerous applications in natural products and synthetic molecules with diverse pharmaceutical properties.Aza-fused heterocycles have divulge potential pharmacological properties such as anti-oxidant, anti-tumor, anti-depressant and anti-coagulant.[3]Synthesis of fused aza-heterocycles *via* transition metal catalyzed oxidative C-C and C-N bond formation is an emerging and effective protocol in synthetic chemistry.[4]Because of enormous importance of coumarin and quinolinones derivatives in biological and pharmaceutical chemistry and our interest in developing a new protocol for the synthesis of fused aza-heterocycles,herein, we report a facile approach to incorporate another aza-heterocyclic moiety into coumarins and quinolinones through one pot sequential Ullmann type C-N coupling followed by Pd-catalyzed oxidative cross dehydrogenative coupling (**Scheme 1**).



Scheme 1.Synthesis of coumarin and quinolinones fused aza-heterocycles

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P-80

One-pot Sequential Knoevenagel Condensation and Oxidative Cross Coupling Reactions: Direct Accessof Imidazopyridine Fused Indoles

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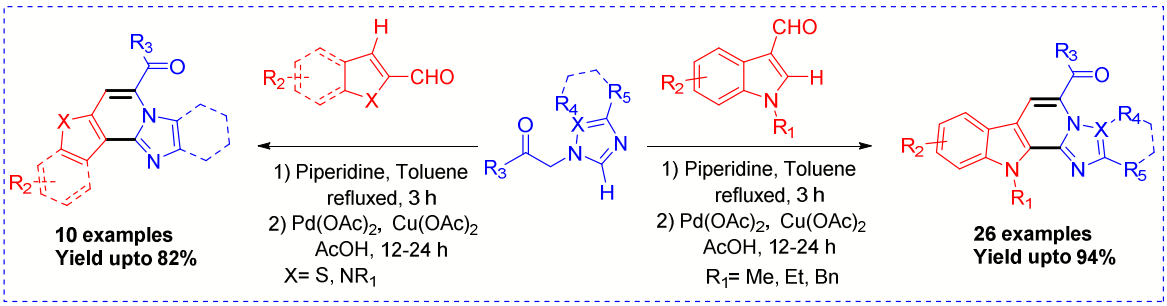
Abstract: Transition metal catalyzed oxidative C–C/C-heteroatomcross couplinghas been emerge a powerful tool for construction of polyheterocycles in moderen era because of their step- or atom-economy and environmental-friendly nature as compared to traditional cross coupling reactions. The construction of targeted C–C bond to access fused aza-heterocycles by usingsimple commercial starting materials is a challenging task to the organic chemist.[1]

In view of the importance of indole fused scaffolds in medicinal chemistry,[2]and our ongoing interest to develop new methodology for the construction of aza-fused heterocycles.[3] Herein, we wish to report a simple and efficientone-pot sequential strategy forsynthesis of imidazopyridine fused indoles in*via*Knoevenagel type condensation ofactivemethylene azoles and*N*-substituted-1*H*-indole-3-carboxaldehydesfollowed byPd(II)-catalyzed intramolecular cross dehydrogenative coupling (**Scheme 1**).[4]



Scheme 1: Synthesis of imidazopyridine fused indoles

References:

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P-81

An Efficient One-Pot Synthesis and Exploration of Photophysical Properties of Triazole Tethered Boron-dipyrromethenes

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Abstract: Dipyrromethane and Boron-dipyrromethenes (BODIPYs) have been continue to receive tremendous recognition owing to their simple structure, interesting and advantageous spectroscopic properties and to be useful as versatile fluorescent probe dyes in biotechnology field [1-2]. They have good solubility and stability against light and chemicals, exhibit relatively high molar absorption coefficients and fluorescence quantum yields[3].Moreover, spectroscopic and photophysical properties of BODIPYs can be fine-tuned by functionalizing the *meso* or α,β-peripheral positions of core dipyrromethene [4-5].In continuation of our efforts to identify effective photosensitizers and fluorescent probes, we have developed a facile synthetic protocol to access diverse 1,2,3-triazoles tethered BODIPYs. In view of the importance of dipyrromethane and functionalized BODIPYs, we have prepareda novel series of α,β- substituted triazolo appended BODIPYsand investigated their photophysical properties. Formation of triazole tethered dipyrrolesinvolvesthe initial reaction of BODIPYswith iodine(III) reagents and sodium azideto *in situ* generate BODIPYs azideswhich was subjected to copper-catalyzed azide−alkyne cycloaddition. Newly prepared BODIPYs derivative were fully characterized by NMR (^{1}H &^{13}C) and HRMS-TOF mass spectral data. Some of the prepared BODIPYs derivatives were found to display interesting absorption and emission properties. Synthesis, characterization and photophysical studies of the triazole appended BODIPYs will be highlighted in the conference presentation.

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P-82

Efficient Synthesis and Identificationof Indolyl-α-keto-1,3,4-oxadiazoles as Tubulin Interacting Potent Anticancer Agents

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Abstract: Microtubules cytoskeleton are composed of α and β tubulin hetero dimers [1]. They play key role in numerous biological functions such as intracellular transport of cellular components during interphase, developing the mitotic spindle throughout the cell division as well as maintaining the cell motility and cell morphology. For this reason, chemical agents that interfere with microtubule cytoskeleton functions are found to have broad spectrum of anticancer activity [2]. In the past few years; indole has been introduced as a privileged moiety in the field of drug discovery and development [3]. Among the indole analogues, aroylindoles, arylthioindoles, indibulin, 2-aryl-4-benzoylimidazoles, diaryl indoles, have been reported to show significant inhibition of tubulin assembly [4]. In order to discover some potent indole-based anticancer agents, recently we identified various indolylazoles with enhanced cytotoxicity, for example indolylisoxazolines, bis(indolyl)ketohydrazide-hydrazones, 5-(2'-indolyl)-thiazoles, 2-arylamino-4-(3'-indolyl)-thiazole [5]. In continuation of our efforts to discover potent cytotoxic indoles, in the present work we have designed and synthesized a diverse series ofindolyl-α-keto-1,3,4-oxadiazoles by using molecular iodine-mediated oxidative cyclization of readily available hydrazide-hydrazones.Synthesized indolyl-keto-oxadiazoles were adequately characterized by using various spectroscopic techniques (IR, NMR and HRMS) and screened *in-vitro* against various cancer cell lines such as human lymphoblast (U937), leukemia (Jurkat & SB) and human breast (BT474).Some of the compounds showed potent *in-vitro* anti-proliferative activity against a panel of cell lines with IC_{50} values in low micromolar range. Also, molecular docking studies of the most potent compound suggested a potential binding mode at the colchicine binding site.

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P-83

Copper (II) catalyzed oxidative chemo- and regioselective dearomatization/ dimerization of 2-arylindoles

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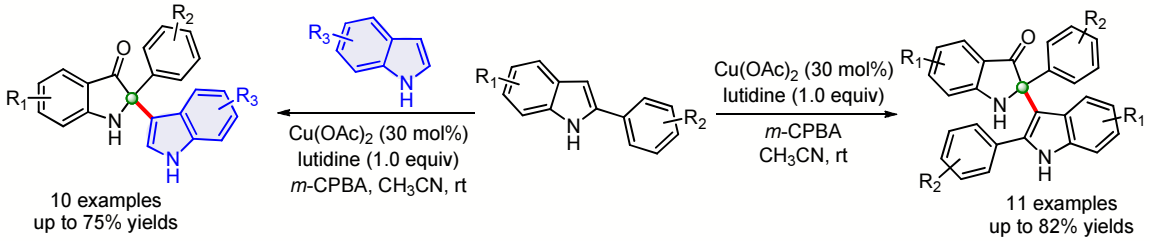
Abstract: An oxidative dearomatization/dimerization process of 2-arylindole via a unique pathway involving Cu(II)-catalyzed C−3 oxygenation by using *m*-CPBA and lutidine as a base has been developed. This protocol provide aneasy access to a series of bisindolin-3-ones bearing a C-2quaternary centre, a motif present in various indole alkaloids, through chemo- and regioselective transformations.



Scheme-1: Rapid synthesis of 2-phenylindolin-3-one derivatives

We have successfully developed an efficient method for the synthesis of 2-phenyl-2-(2-phenyl-1*H*-indol-3-yl)indolin-3-ones and 2-(1*H*-indol-3-yl)-2-phenylindolin-3-ones using easily available and non-toxic materials, eliminating the use of hazardous and expensive reagents used in previous methods. By using effortless strategy which provides convenient access to indolin-3-ones bearing C-2 quaternary centre in high yields. This method is practical and unpretentious as it can be easily scaled up and will be presented.

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P-84

Asymmetric synthesis off used 1,2-dihydropyridines *via*metal-free formal[4+2] cyclo addition between aqueousglutaraldehyde and dibenzo[*b,f*][1,4]oxazepineimines

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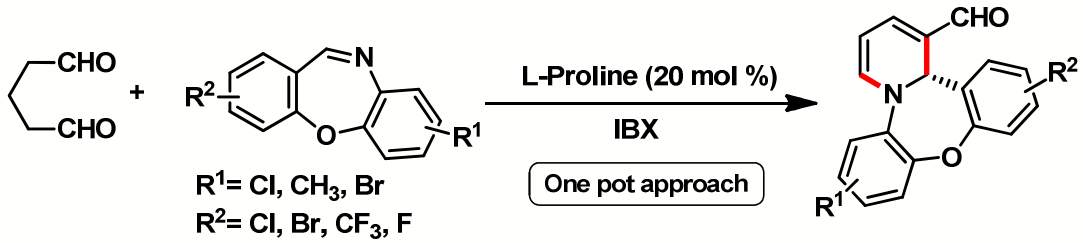
Abstract: Dihydropyridines (DHPs) are frequently encountered in natural and synthetic compounds that possess many interesting biological activities.[1]On the other hand, The dibenzo[b,f][1,4]-oxazepine scaffolds are core structures in numerous biologically active compounds.[2]Some of these derivatives also exhibit anti-HIV, anti-tumor and anti-inflammatory activities.[3]Thus, the 1,2-Dihydropyridine-fused dibenzo[*b,f*][1,4]oxazepines might exhibit impressive bioactivities. In continuation of our interest in organocatalyzed reactions,[4] we recently developed an efficient organocatalytic asymmetric method for the synthesis of 1,2- Dihydropyridines (DHPs) using aqueous glutaraldehyde and imines with high yields and excellent enantioselectivity.[5]Here, we present a new method for the asymmetric synthesis of fused 1,2-dihydropyridines via metal-free formal [4+2] cycloaddition between aqueous glutaraldehyde and dibenzo[*b,f*][1,4]oxazepine imines**(Scheme 1).**



Scheme 1: Organocatalytic asymmetric synthesis of dibenzo[*b,f*][1,4]oxazepinefused 1,2-DHPs

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P-85

A simple entry to novel tetracyclic oxazepine-fusedpyrroles *via* metal-free [3+2] annulation between dibenzo[*b*,*f*][1,4]oxazepines and aqueous succinaldehyde

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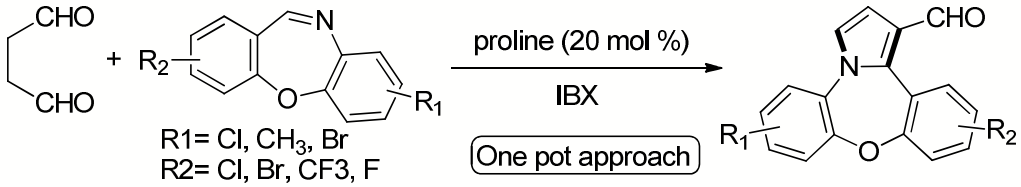
Abstract: Pyrrole moiety present in numerous natural products with biologically activities such as antiviral, antitumor, antioxidative, anti-inflammatory activities.[1]On the other hand,dibenzo[*b*,*f*][1,4]oxazepine (DBO), as well as their derivatives, are regarded as "privileged scaffolds" in medicinal chemistry.[2] In particular, heterocycles *ortho*-fused dibenz[*b*,*f*][1,4]oxazepines, resembles the tetracyclic anti-depressants (TeCAs), with similar and interesting bioactivities.[3]Thus, the pyrrole-fused dibenzo[*b*,*f*][1,4]oxazepines might exhibit impressive bioactivities. In continuation of our interest in organocatalyzed reactions,[4] we recently reported an organocatalytic multicomponentmethod for the synthesis of pyrrole-3-carboxaldehydeusing aqueous succinaldehyde and imines with high yields [5]. Here, we present a new method for the synthesis of tetracyclicoxazepine-fused pyrroles under metal-free condition fromdibenzo[b,f]-[1,4]oxazepines and aqueous succinaldehyde **(Scheme 1).**



Scheme 1: Organocatalyticone-pot synthesis of tetracyclic fused pyrroles.

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P-86

Additive-Driven Rhodium-Catalyzed [4+1]/[4+2] Annulations of *N*-Arylphthalazine-1,4-dione with *α*-Diazo Carbonyl Compounds

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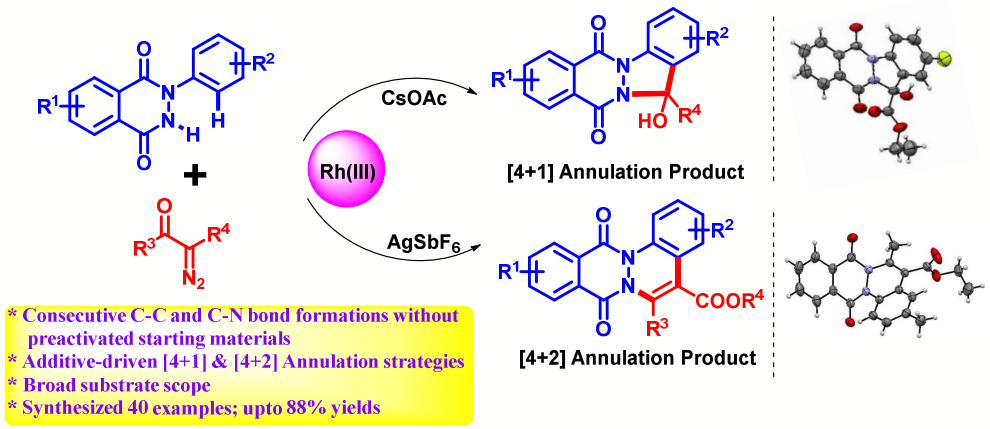
Abstract: Transition-metal-catalyzed oxidative annulation *via* C–H activation involving directing groups is among the most acclaimed approach for sequential C–C/C–N bond formations.[1,2] In recent years, a number of transition-metal-catalyzed annulation protocols have been developed on *2*-arylphthalazine-1,4-dione using different coupling partners such as internal alkynes, propargyl alcohols, alkenes *etc*, for constructing fused-phthalazines.[3,4] However, annulation using carbene insertion generated through the decomposition of *α*-diazo carbonyl compounds on 2-arylphthalazine-1,4-dione has not been explored to date. Herein we present a Rh(III)-catalyzed strategy involving [4+1] annulation of 2-arylphthalazine-1,4-diones with *α*-diazo carbonyl compounds, accessing a series of unprecedented hydroxy-dihydroindazolo-fused phthalazines in good-to-excellent yields.[5] By varying the additive, phthalazino-fused cinnolines were synthesized under Rh-catalyzed conditions *via* [4+2] annulation between same starting materials. Notably, both the strategies showed good functional group tolerance and high atom-efficiency. A series of compounds were synthesized and characterized using ^{1}H NMR, ^{13}C NMR, HRMS and single crystal XRD.



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P-87

Iridium-Catalyzed [4+2] Annulation of 1-Arylindazolones with *α*-Diazo Carbonyl Compounds: Access to Indazolone-fused Cinnolines

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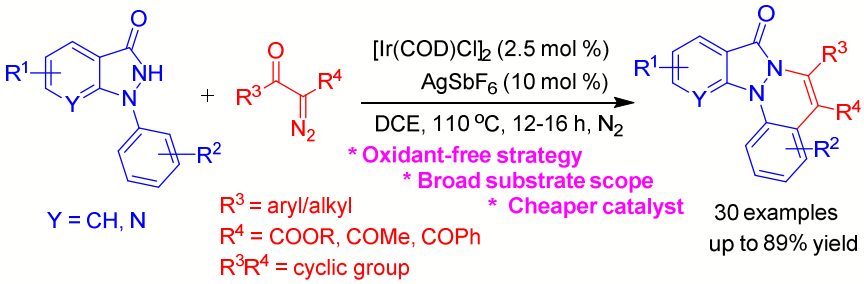
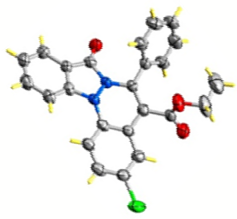
Abstract Indazole framework is a ubiquitous privileged unit found in many natural products, and its synthetic analogs are widely implicated as pharmaceuticals, catalysts, and functional materials due to their diverse physical and chemical properties.[1,2] Accordingly, various synthetic approaches to access functionalized and fused indazoles have been established.[3,4] In specific, noticeably contributions have been documented towards the synthesis of fused indazoles *via* various transition-metal catalyzed strategies in the past decade.[5,6]

In spite of previous synthetic wisdom collated, developing efficient synthetic strategies for the construction of fused indazoles are still of great interest. Under this realm, an efficient one-pot Iridium-catalyzed strategy for the synthesis of indazolone-fused cinnolines has been developed by [4+2] annulation of 1-arylindazolones and *α*-diazo carbonyl compounds *via* sequential C-H activation/carbene insertion/cyclization in a tandem fashion. The protocol showcased excellent tolerance towards electron-withdrawing as well as electron-donating functional groups on 1-arylindazolone. The methodology was also found to be workable with cyclic *α*-diazo carbonyl compounds.





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P-88

PEGylated block-copolymer: A nano-drug vehicle as a drug candidate in Alzheimer's disease

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Abstract: In the field of drug development against Alzheimer's disease, a new drug candidate is coming up almost every day, [1-3] but a successful one is still missing showing a positive result in human phase trials [4-6]. Since its discovery by Dr.Alois Alzheimer's in 1906 [7], the pathophysiology of the disease remains very dynamic addressing mainly three hypotheses, *viz*, amyloid cascade hypothesis, taupathy and very recent mitochondrial cascade hypothesis[8-10]. On the other hand, a targeted drug delivery-vehicle development is always being in the limelight in the field of neurotherapeutics [3]. Keeping it in mind, we tested a side chain tripeptide (Leucine-valine-phenylalanine) based PEGylated block-copolymer as a drug candidate against the fibrillization inhibition of amyloid beta 1-42 ($A\beta_{42}$) of the Alzheimer's disease. Here, the PEGylated block copolymer with some modification of a previously reported compound [11] has been proved to be a promising drug candidate via Thioflavin-T fluorescence assay, Dynamic light scattering analyses, microscopic image documentations and *in vitro*cellularassays and so on. Through our current study we are reporting a modified nano-drug vehicle as a drug candidate itself which may enlighten the alternative drug development against Alzheimer's disease.

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P-89

Structure and solution behaviour of differently linked diubiquitins Sudipa Mondal, Sudit

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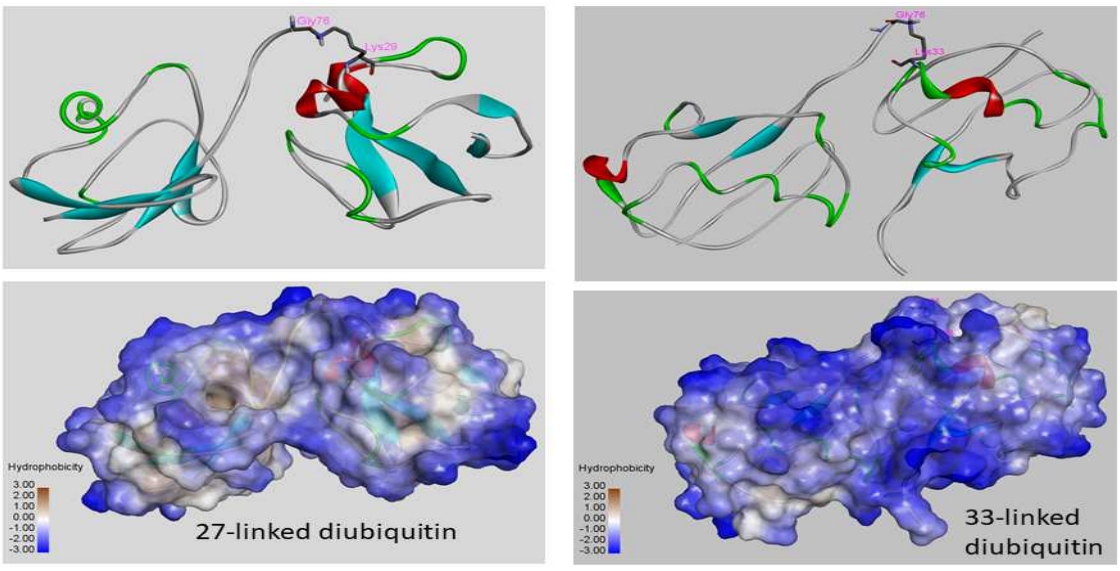
Abstract: Ubiquitination, the posttranslational modification of proteins with one or several ubiquitin molecules can alter the fate, activity, localization and protein-protein interactions of the modified protein. Ubiquitin is a compact 76 amino acid protein that is highly conserved from yeast to mammals and forms distinct isopeptide linkages between one of its seven lysines or the N terminus of the proximal ubiquitin and the C-terminal carboxyl of the distal ubiquitin. Different outcomes are achieved depending on the identity of the ubiquitin linkage. The effect of ubiquitin modification is read out by interactions of ubiquitin or ubiquitin chains with target proteins. Thus, the conformational differences and specificity of the various ubiquitin linkages have been of great interest to biologists in many disciplines [1, 2]. The solution behaviour for all ubiquitin linkages is more complicated than static crystal structures would suggest. The solution behavior of isolated linkages is best explained by multiple conformations [3, 4, 5]. K48-, K63-, and K11-ubiquitin linkages have well-established biological roles, whereas K27-, K-29 and K-33 linked ubiquitins are much less characterized both biologically and structurally. Here we have studied and explored the dynamic behaviour of all the diubiquitins and 1st time predicted the structure of K29-linked and K3- linked diubiuitin in solution. We have also perdicted the structure of other di-ubiquitins and compared with their crystal structure. Dynamic nature, conformational behaviour and their comparison amongst all the diubiquitins were done also.



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P-90

Enantioselective LCMS Method Development and Validation of Pregabalin

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Abstract: Pregabalin (S-enantiomer) has approximately 10-times more affinity for alpha2-delta binding than the R-enantiomer [1]. Therefore, only (S)-enantiomer is applied for clinical use and (R)-enantiomer is considered as an optical impurity and its concentration needs to be monitored and control in the final product. In order to increase awareness towards biologically important isomers, the US Food and Drug Administration has issued certain guidelines for the marketing of racemic compounds [2]. This new trend resulted in the determination of chiral impurities at a concentration below 0.1 % and this place heavy demand on the chiral analytical methods [3-4]. There are various reports for the direct estimation of pregabalin in biological samples using hyphenated LC-MS/MS. There are many laboratories which have only single quadrupole LC-MS and can not procure such expensive LC-MS/MS. There is no published report for direct chiral estimation of pregabalin in formulation sample using single quadrupole LC-MS.
The present work deals with the systematic method development for the direct separation of Pregabalin and (R) -enantiomer using macrocyclic glycopeptide chiral stationary phase (CSP). The method was validated for the parameters; eg. specificity, linearity, accuracy, precision, limit of detection and quantification.

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P-91

Thermophysical and Spectral Study of Ternary Mixtures of β-pinene with N,N-DMF and Aromatic Hydrocarbons

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Abstract: The investigation of association in between the molecules in solution state have shown a need for approximations for the thermochemical properties of a ternary solvent systems.The interaction between solvent and solute molecule may result in some gross modifications of their activities, reactivity and Properties. In this study,density (ρ), refractive index (n_D) of Ternary mixtures of β-pinene with N,N-DMF and aromatic hydrocarbons has been measured over the entire composition range expressed by mole fraction (x_1& x_2) and volume fraction (ϕ_1&ϕ_2) of the β-pinene at 303.15, 308.15 and 313.15 K at atmospheric pressure. The FT-IR measurements were carried out at 298.15 K. From the experimental data, excess molar volume (V^E) and deviation in refractive index (Δn_D) and have been calculated and had fitted to Redlich-Kister polynomial equation. The excess or deviation parameters were plotted against mole fraction or volume fractionof the β-pinene over whole composition range. The observed negative or positive values of excess or deviation parameters were explained on the basis of the intermolecular interactions present in these mixtures. The position, pattern and intensity of band as per FT-IR data strongly supports the conclusion that molecular interactionshave taken place, it is also supported by the V^E and Δn_D data.

Keywords: Density, Excess molar volume, Refractive index, Molar refraction,Mixing rules, FT-IRspectroscopy.

P-92

'One-Pot Synthesis of Fully Substituted Pyrimidines Using Amidine and Ketene dithioacetals as Synthons'

Mayur Shiyal, Khushbu Dodeja, Prof. Y. T. Naliapara*

Abstract: A simple, convenient and efficient one pot synthesis of fully substituted pyrimidines was developed by cyclocondensation of α-oxo ketene dithioacetals with amidine in the presence of potassium carbonate in good yield. Structures of all the newly synthesized compounds were elucidated by elemental analysis and spectral analysis.

Keywords: non metallic synthesis of pyrimidines, high yield with using potassium carbonate

P-93

Natural products approach for the synthesis of quinazoline hybrids as potent antileishmanial agents

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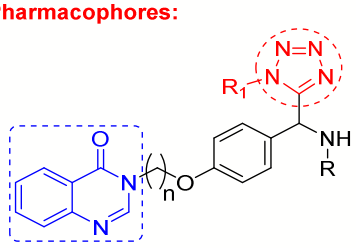
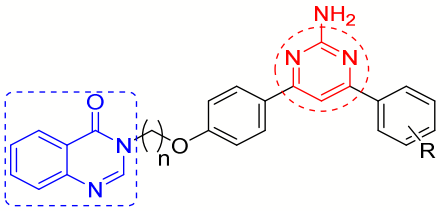
Abstract: In an attempt to discover novel antileishmanial Quinazolinone hybrids, a series of 23 compounds were synthesized utilizing the Ugi multicomponent reaction and some of them were found to be active in antileishmanial screening. Most of the screened derivatives exhibit significant in *vitro* activity against antiamastigote activity with **IC_{50}**value in the range of **3.66** and **6.86 µM.** of*L.donovani*and cytotoxicity against the J774A.1 cell line. Their activity is comparable with standard drugs miltefosine and sodium stibogluconate. The potential active analogue was further studied in *vivo* against the L.donovani/golden hamster model at a dose of 50 mg Kg/day through intraperitoneal (I.P.) route for 7 days which displayed **13±8.66, 20.41±5.57** inhibition, in parasite multiplication together with its low toxicity against macrophages.

Key words: Novel antileishmanial Quinazolinone hybrids

Pharmacophores:



R_1= *tert*-butyl
R= Isopropyl, n=4, (IC_{50}= 3.66 µM)
R= Isopropyl, n=5,(IC_{50}= 6.86 µM)
(SI= 35.10, 28.30)



R= *p*-methoxyphenyl *p*- cholorophenyl, *p*-F (n= 3-5), ND

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P-94

Open Flask, Clean and Practical Protocol for Diastereoselective Syntheses of Oxindole Containing Phosphinoyl Compounds under Catalyst-Free and Solvent-Free Conditions

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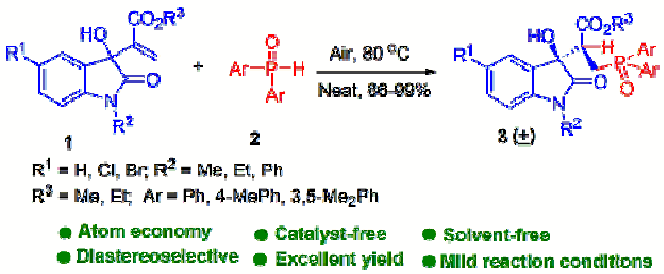
Abstract: Considering the importance of organophosphorus compounds in organic synthesis, organometallic chemistry, medicinal chemistry, chemical biology, and material science,the development of cleaner and more efficient methods for their synthesis holds particular significance in recent years.[1]An open flask, practical C-P bond formation between oxindole containing allyl alcohols and phosphorous surrogates under catalyst-free and solvent-free conditions is described. The C-P bond formation is completely diastereoselective and amenable to a variety of multifunctional allyl alcohols under the reaction conditions employed, providing the desired products in excellent yields.[2]



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P-95

Room Temperature, Open Flask C-P Bond Formation on Water Under Catalyst-Free Conditions

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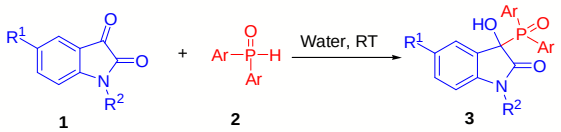
Abstract: Organophosphorus compounds play important role in the organic synthesis, organometallic chemistry, medicinal chemistry, chemical biology, and material science.[1] More importantly, □-hydroxy and □-amino phosphonic acids have found to play the vital role in the pharmaceutical industry, biophosphate mimics, antibiotics, antivirals, and antitumor agents.[2]A catalyst-free C-P bond formation under open flask at room temperature between isatin derivatives and phosphorus surrogates on water is described. Isatin derivatives possessing different substitutes underwent C-P coupling reaction with a variety of phosphine oxides under the reaction conditions employed, provided the desired products up to quantitative yields.[3]



R^1 = H, Cl, Br, NO_2; R^2 = H, Me, Et, Ph
Ar = Ph, 4-MePh, 3,5-Me_2Ph, OPh

100% Atom economy **Catalyst-free** **Green Synthesis**
Room temperature **Excellent yields** **28 Examples**

Reference:

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P-96

Regio- and stereoselective C-S Bond formation uder metal-free conditions

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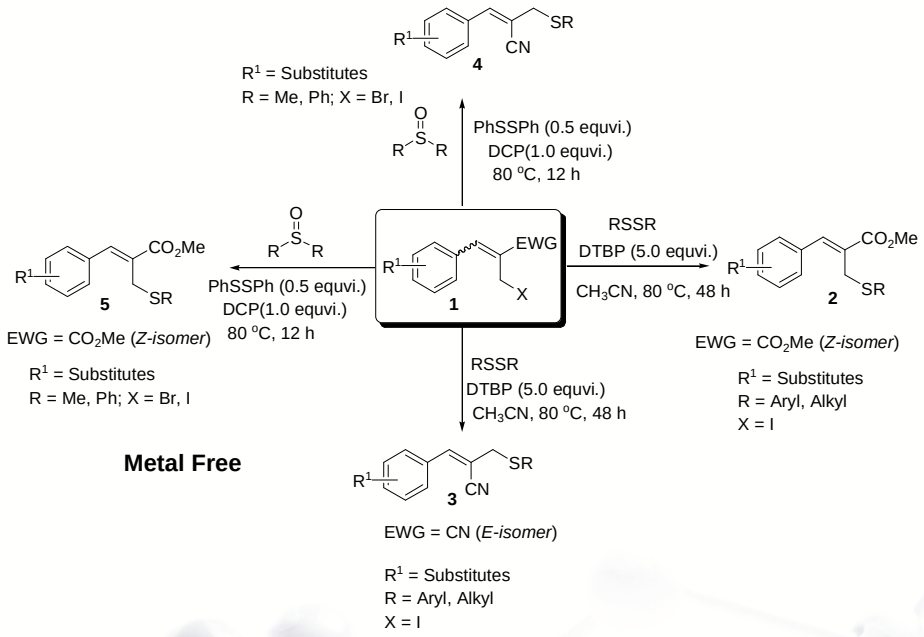
Abstract: Due to their versatile applications inorganic synthesis, pharmaceutical industry and materials science, in recent years various metal catalyzed procedures have been devloped for the syntheis of thioethers.[1] At present, the C-S cross coupling reactions between halides and sulphur surrogate under metal free conditions have emerged as a fantastic tool for the syntheis of thioethers and thioesters.[1] A solvent controlled C-S coupling reaction between allyl iodides/bromides and aryl or alkyl disulfides as coupling partnerunder metal free conditions is described which provided a facile methodology for the regio and stereoselective synthesis of allylic thioethers.[2]When the reactionswere carried out in DMSO/DPSO, the *S*-methylation/phenylation occoured whereas in CH_3CN the corrosponding aryl/alkyl allyl thioethers were obatined. The allyl iodides/bromides[3]possesing different stereochemistry (*E*&*Z*) underwent C-S bond formation with a variety of disulfides provided the resulting allyl thioethers in good to excellent yields.



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P-97

Tandem Michael addition of amines to substituted maleimide

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Abstract: The Michael addition reaction has been extensively used for making C-C and C-X (X= N, O, P, S) bonds in organic synthesis. The mild reaction conditions, possibility of using a wide variety of Michael donors including the chiral ones enhance its utility. The aza-Michael reaction can be used as an important synthon to synthesize β-amino carbonyl compounds, which are used as chiral auxiliaries and bioactive natural products.

We have recently reported experimental and theoretical explanation of the aza-Michael additions of amines with dimethyl acetylenedicarboxylate[1]. In continuity of this, we carried out aza-Michael addition reaction of some amines namely diethylamine, pyrrolidine, piperidine with substituted maleimides.The products have been studied theoretically as well as experimentally. Characterization of all the products has been done by ^{1}H NMR, ^{13}C NMR, IR spectral studies.

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P-98

ZnO assisted photocatalytic degradation of explosive picrate in the presence of UV light

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Abstract: The Photocatalytic degradation of metal - picrate in aqueous solution using ZnO photocatalyst has been carried out. The absorbance of photocatalytic reaction at different time intervals has been observed spectrophotometrically. Rate of reaction was observed for different parameters like concentration, effect of amount of photocatalyst, pH, light intensity and band gap.

Keywords: Photocatalysis, Metal-picrate, zinc oxide.

P-99

Synthesis of highly functionalized pyrido[2',1':2,3]imidazo[4,5-c]isoquinolines through the sequence of Groebke-Blackburn-Bienayme and isocyanide insertion reaction under aqueous condition

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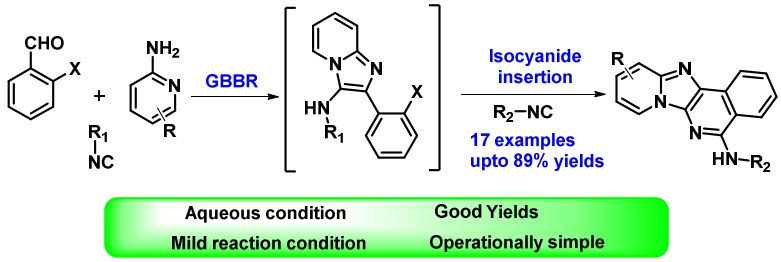
Abstract: Green and efficient protocols are recognized by the synthetic chemist to rapid access biologically active heterocycles. In this perspective, research involving the synthesis of organic heterocycles in water as a reaction medium has been attracted considerable attention in recent years. [1]

Aza-polyheterocycles and its analogs are widely distributed among natural products, pharmaceuticals, and functional materials. [2] These aza-polyheterocycles molecules possess a wide range of biological and pharmaceutical activities such as antifungal, antibacterial, antineoplastic, anticancer, antiplasmodial and DNA intercalators. [3]

In the light of above fact, herein we report an efficient two step process for the synthesis of biologically relevant highly functionalized pyrido[2',1':2,3] imidazo[4,5-*c*]isoquinoline in aqueous medium through an Ugi type 3-component (Groebke-Blackburn-Bienayme reaction) (GBB) reaction/Palladium catalyzed isocyanides insertion reaction in good to excellent yields.



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P-100

Chemoselective synthesis of *m*-teraryls through ring transformation of 2*H*-pyran-2-ones by 2-(1-arylethylidene)-malononitriles

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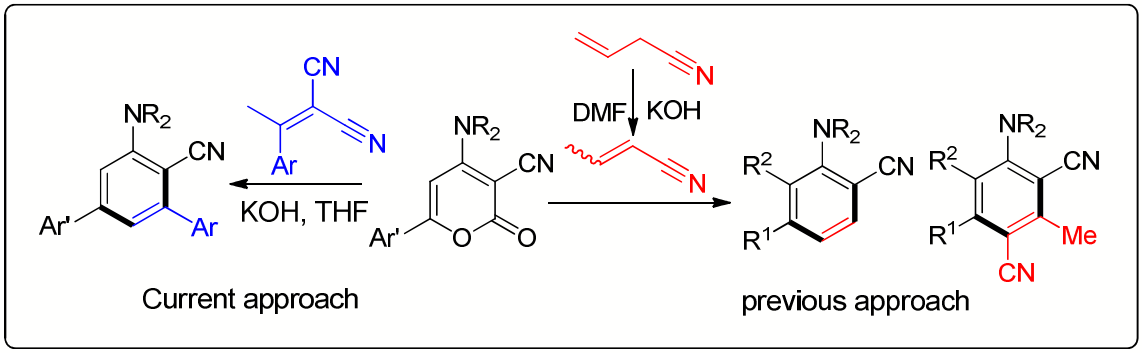

Abstract: We have developed a simple, efficient and chemoselective approach for the synthesis of *m*-teraryls by the reaction of 6-aryl-2-Oxo-4-(*sec*.amino)-2*H*-pyran-3-carbonitriles and 2-(1-arylethylidene)malononitriles under basic condition. We used 6-aryl-2-oxo-4-methylsulfanyl-2*H*-pyran-3-carbonitriles as a precursor and successfully afforded 5'-methylsulfanyl-[1,1';3',1"]teraryl-4'-carbonitriles. We tried to understand the difference in the reactivity of structurally symmetrical allyl cyanide, 2-cyanomethylbenzonitrile and 2-(1-arylethylidene)malononitrile[1-3]. The structure of the 4"-methyl-5'-(piperidin-1-yl)-[1,1':3',1''-terphenyl]-4'-carbonitrile was confirmed by single crystal X-ray diffraction analysis.

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P-101

Computational Insight to Regioselective Synthesis of Pyrrolopyridine Derivatives and Biomolecularintercation

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Abstract: Naturally occurring bioactive alkaloids incorporating pyrrolopyridine nucleus are one of the important class of natural products. Several representatives isolated from plants, insects and microorganisms have been proved to be an effective targets in drug designing. Hence, efforts have been made to synthesize pyrrolopyridines having variety of substitution patterns with potential importance in both synthetic and medicinal chemistry. In the present study, [3+2] cycloaddition reaction of 1-(2-ethoxy-2-oxoethyl)-3-methylpyridinium bromide with symmetrical DMAD and unsymmetrical methyl propiolate has been carried out. The reaction mechanism has been investigated by computational calculations at DFT (B3LYP/6-31+g**) level to examine regioselectivity. The major and minor regioisomershave been predicted by calculating activation energy barrier of the transition state at the same level. The results revealed that with DMAD two regiosomers are possible while with methyl propiolate four regioisomersmay be possible. The computational results have been compared with experimental yields and were found to be in good agreement.Biomolecular interactions of selected representatives have been identified using Docking studies.

P-102

Phytochemical investigation of Petroleum ether seed extract of *Abrus precatorius*

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Abstract: *Abrus precatorius*, popularly known as Rati in Hindi, Crab's eye in English and Gunja in Sanskrit, belongs to family Fabaceae. *Abrus precatorius* is one of the major ingredients of some of the Ayurvedic hair growth promoting formulations. In view of our interest in natural hair growth promoter, we have analyzed its seed extracts using Gas Chromatography-Mass Spectrometry and screened it for its hair growth promoting activity. Isoflavonoids, flavonoids, proteins, alkaloids, carbohydrates, and triterpenoids were isolated from its seeds by researchers. GC-MS analysis of the petroleum ether extract of seeds of this plant showed the presence of cis-vaccinic acid,1,2,3,4-bis-o-ethyl borandyl-6-(diphenylphospheno)-6-desoxy-alpha-d-glactopyranose, stigmasta-5,22-dien-3-ol, Pentadecanioc acid, cyclic 1,2-ethanediyl acetal, (5.alpha.)- Cholestan-3-one, 1,3-dimethyl-benzene , (3.beta.)-Ergost-5-en-3-ol, and 5-Cholesten-24.beta.-ethyl-3.beta.-ol.Hair growth promoting of the extract and its major compound is under progress.

P-103

Copper–Catalyzed 1,3-Dipolar Cycloaddition of IsoquinoliniumYlide

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Abstract: 1,3-Dipolar cycloaddition reaction of various cycloiminiumylides is a well known method to obtain variety of bridgehead *N*-heterocycles. Cycloaddition reactions of cycloiminiumylides, such as pyridinium and isoquinoliniumylides with unsymmetrical dipolarophiles follow stereo and regioselectivity. Copper catalyzed stereoselective 1,3–dipolar cycloaddition of isoquinoliniumylides and electron deficient alkenes has been investigated under mild conditions. The pyrroloisoquinoline derivatives incorporating bridgehead nitrogen were obtained in moderate to high isolated yields (65-82%) with excellent stereoselectivites. Role of copper ions in feasibility of reaction has been investigated computationally.

P-104

Recent Advances on peroxide catalyzed C-S Bond formation under metal-free conditions

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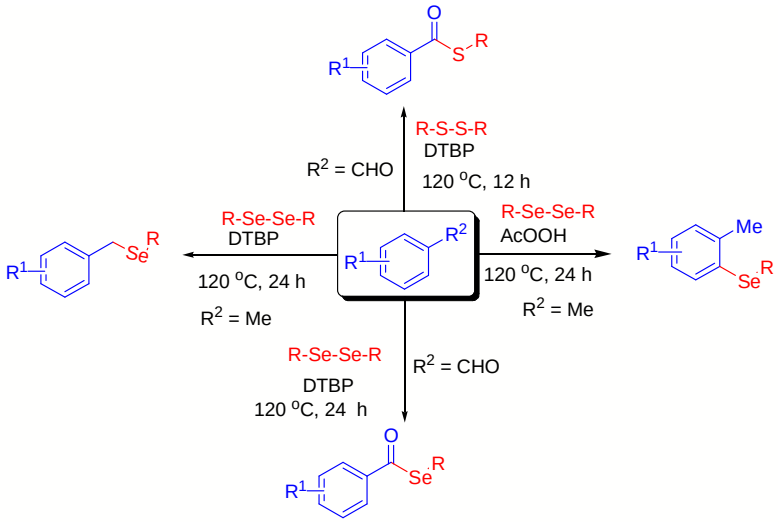
Abstract: Recently, the metal free organic transformations especially *via* peroxide catalysis emerged as interesting substitute for the metal catalysed coupling reactions. Various C-C, C-S, C-N, C-O, C-Se bond forming reactions have been carried out under peroxide catalysis.[1]These reactions proceed via radical mechanism. An Oxidant dependent metal free and solvent free thiolation/selenation of methyl arenes/aldehydes using disulfide/diselenides as source of sulphur/selenide has been described. The resultant thioether, selenide ethers, thioesters were obtained in good to excellent yield.[2]



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P-105

GC-MS Analysis and Antimicrobial Activity of an Anti-dandruff botanical : *Brassica juncea*

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Abstract: Indian mustard (*Brassica juncea*) popularly known as Rai, is one of the most important oilseed crop of Brassicaceae (cruciferous) family. A paste of Rai and *Buchanania lanzan* is topically applied on the head to prevent dandruff. In view of our interest in antidandruff botanicals we have analyzed its seed extracts using Gas Chromatography–Mass Spectrometry and screened it for its antimicrobial activity. GC-MS analysis of the petroleum ether extract revealed the presence of 38 compounds. (2Z, 13E)-2, 13-Octadecadien-1-ol, hexadecanoic acid, cis-.beta.-farnesene, 3[(trimethylsilyl)oxy]cholest-5-ene, 1H-benzocycloheptene, 2,4a,5,6,7,8-hexahydro-3,5,5,9-tetramethyl-, (R)-, ergost-5-en-3beta-ol, n-tetra tetracontane and n-tetracontane were identified as major compounds. The results of the antimicrobial study suggested that ethyl acetate extract exhibits maximum antimicrobial inhibition activity against tested bacteria *Escherichia coli*, *Staphylococcus aureus* and fungus *Malassezia furfur*. Pet-ether extract of the plant showed moderate antifungal activity, while ethyl acetate, ethanol, and methanol extracts showed significant activity against *Candida albicans*.

P-106

$^{18}F/^{11}C$-PET Radiochemistry Strategic challenges: Transforming Bench to Bedside

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Abstract: In the field of radiopharmaceutical research, the development of new radiochemistry methods has been one of the major driving forces for positron emission tomography (PET) imaging during the past decade. The use and availability of the positron emitters[1-4] C-11, F-18, Ga-68, Cu-64, or Zr-89, to name a few, have enormously increased and, especially in terms of chemo-selectivity and radio labelling efficacy, significant progress has been made. The low energy nuclear reactor also called Cyclotron played a major role in providing the medically relevant radioisotopes on site for the treatment and diagnosis of patients. One of the most useful and prevalent clinically useful radioisotopes is of Fluorine or carbon i.e., F-18/C-11. The field of F-18 chemistry embedded with variety of synthetic strategies such as click chemistry-based labelling methods, the use of the silicon-fluoride acceptor reagents, and Al-FNOTA complexes offer an even more simplified strategy to introduce F-18 into bio molecules. These techniques facilitate the syntheses of radiotracers for PET imaging studies and thus accelerate their pronounced use in clinical and preclinical studies.

We at SGPGIMS with 18 MeV cyclotron having capacity to produce the various clinically and preclinical relevant positron emitters radio isotopes such as C-11, F-18, Cu-64, N-13, O-15, I-123, I-124 or Zr-89. These radio-isotopes are used to synthesise different radio-pharmaceuticals such as [^{18}F]-FDG, [^{18}F]-FLT, [^{18}F]-FES, [^{11}C]-Methionine for, [^{18}F]-NaF, ^{13}N-NH_3 treatment and diagnosis using different chemical insertion protocols and methods. In this presentation we are presenting our few such strategies which transfer organic molecules from bench to clinical studies.

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P-107

BIOANALYTICAL METHOD AND FORCED DEGRADATION STUDIES OF CHLORDIAZEPOXIDE AND TRIFLUOPERAZINE COMBINATION BY RP-HPLC AND LC-Q-TOF

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Abstract: Bioanalytical methods can be applied to study clinical pharmacology, toxicology principles, thus playing a vital role in better interpretation of bioequivalence, pharmacokinetic, toxicokinetic studies and therapeutic monitoring of drug. On the other side, stress studies are designed to generate product-related variants and develop analytical methods to determine the degradation products formed during accelerated pharmaceutical studies and generated impurities may further reduce the quality or safety aspects.

The RP-HPLC method was developed for the simultaneous estimation of both entities in simulated plasma using protein precipitation technique of bioanalytical sample preparation as per ICH guidelines (ICH Q2B_R1). The method was found to be linear (r^2= 0.9997 & 0.9999), precise, efficient and accurate with high sensitivity (LLOQ – 30ng/mL). The developed method for degradation studies was carried out on an SHIMDAZU LCMS-8030.

The developed bioanalytical method was validated as per bioanalytical guidelines (ICH M10) and can be used in therapeutic drug monitoring units, bioequivalence and bioavailability studies, pharmacokinetic and toxicology studies of CDZ and TFP. The forced degradation studies helped to identify new degradation product and intermediate by the LC-MS fragmentation pattern of both drugs under study.

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P-108

Multi-targeting Combretastatin Inspired Ligands as Potential Anticancer Agents

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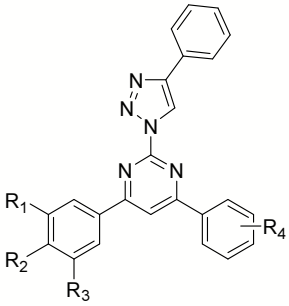
Abstract: Microtubules are one of the prime target for the development of anticancer agents. Combretastatins are one of the few microtubule targeting agents reported to act as vascular disrupting agents (VDA) activity along with cytotoxicity. They acts as vascular disrupting agents as well as mitotic inhibitors[1]. Tumor angiogenic mechanisms are vital for tumor growth and metastasis and targeted by antiangiogenic agents. Angiogenesis is the keystone of tumor progression and metastasis



R_1=R_2=R_3= OCH_3, H
R_1=R_2= OCH_3, R_3=H
R_1=R_3=H, R_2=OCH_3
R_4=H, OCH_3,F, Cl, Br, NO_2

and targeting this within the tumor is regarded as promising strategy for cancer therapy[2].Multi-targeting approach by a single drug molecule represents an efficient, logical and alternative approach to drug combinations. A single agent with VDA, cytotoxicity and antiangiogenic activities could circumvent the various problems associated with single targeted agents or in combination therapy such as tumor cell resistance, toxicity, drug–drug interaction, pharmacokinetic problems of multiple agents.[3] We have designed and synthesized combretastatin inspired multitargeting molecules with pharmacophoric groups to target tubulin protein, VDA and MetAP-2 enzyme (for antiangiogenic activity).

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P-109

Production of biodiesel from a mixed oil of Castor and Mahua

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Dwindling non-renewable energy source has compelled us to look for sustainable energy sources. The availability of oils areregion specific and the amount of a specific oilavailable at one place is not enough to produce biodiesel that fulfilling the requirements. So it is needed to try different mixtures of oil for biodiesel production. Biodiesel(fatty acid methyl esters) was prepared from mixed mahuaoil and castor oilby the process of transesterification, where KOH was used as the catalyst. All the process parameters such as the mahua oil to castor oil mole ratio, methanol to mixed oilmole ratio, catalyst concentration, reaction temperature and the reaction time were analyzed to study the effect on the yield of biodiesel. The effect of the co-solvent, hexane was also studied on the aforesaid parameters. The optimal processconditions for maximum biodiesel yield were,mole ratio ofmahua to castor oil 1:1,methanol to oil mole ratio 16.0:1, reaction temperature 60 °C, catalyst amount 0.4 wt.% and the reaction time 1.5 h. Under the optimum conditions, about 98% yield of biodiesel was obtained.The formation of the biodiesel was ascertained by FT-IR and GC-MS. Also the fuel properties of the biodiesel was analyzed and the performance was studied in I.C. engine.

Key words: Biodiesel, Mahua oil, Castor oil,Transesterification, Mixed oil

P-110

Synthesis, Characterization and Application studies of 4-Aminoantipyrine based Schiff base ligands

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Abstract: Schiff bases ligands and their metal complexes are well known to exhibit antibacterial, antitumor, attractive electronic as well as photophysical properties. In addition, incorporation of a fluorescent moiety in Schiff base derivatives makes them appealing fluorescent probes for metal ions. A series of Schiff base ligands bearing antipyrine moiety were synthesized and characterized by several techniques (UV-Visible, IR, NMR, Fluorescence Spectroscopy). Apart from metal complex synthesis, solvatochromic behaviour and corrosion inhibition tendency of the ligands were studied. The ligands were found to inhibit corrosion of mild steel in acidic solution via adsorption on metal surface. Corrosion inhibition efficiency of around 90% was found in 1N HCl for all the ligands.

Keywords: Schiff Base, Antipyrine, Metal Complex, Solvatochromism, Corrosion Inhibition

P-111

Synthesis and characterizations of some new series of benzimidazole incorporated heteroannulated pyrimidine derivatives for their biological activity

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Benzimidazole is the key core in several bioactive compounds due to presence of imidazole ring which is found in many natural products like histamine, histidine and in nucleic acids and they exhibit varied pharmacological activities such as antioxidants, anticancer, anti-inflammatory, antimicrobial, anti-tuberculosis and antihypertensive [1-3]. In this sense synthetic protocols aiming to achieve this heterocycle core is a continue interest of the pharmacologist in order to bring the new chemical entities as a bioactive lead molecule in a parasitic area as the high mortality rate associated with parasitic diseases is mainly due to the development of parasitic multi-drugs resistant strain. Therefore, drugs currently in the markets are not effective due to their limited pharmacological efficacy and hence, the discovery of new drugs in parasitic area is urgently needed. Keeping in view importance of nitrogen heterocycles in antiparasitic area and our continuous effort to search the novel new chemical entities for their therapeutic potency, recently we have synthesis the some new series of benzimidazolyl incorporated heteroannulated pyrimidine derivatives for their biological activity. In this presentation, the detailed synthetic procedure, isolation and characterizations of the newly synthesized compounds by using elemental and spectral (^{1}HNMR, ^{13}C NMR, EIMS, UV and IR) data analysis will be discussed.

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P-112

One pot synthesis of highly substituted quinolines in aqueous medium and its application for the synthesis of azalignans

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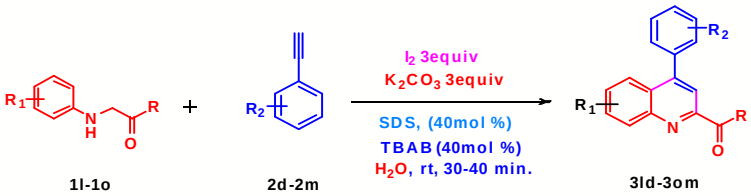
Abstract: A new one-pot method has been developed for the synthesis of highly substituted quinoline derivatives from α-amino ketone derivatives/glycine esters/ glycine amide and aromatic/aliphatic alkynes/alkenyl esters using molecular I_2, K_2CO_3 and tetrabutylammonium bromide (TBAB) and sodium dodocyl sulphate (SDS) surfactant combination in water at room temperature within 30-50 min. in moderate to good yields. This protocol has advantages like oxidant free, aqueous medium, operationally simple, tolerates various substrates, and useful for the synthesis of bioactive azalignans.



Keywords: Phenyl-2-(phenylamino)-ethan-1-one (α-amino ketone), alkyne, iodine, K_2CO_3, sodium dodecyl sulphate, tetrabutyl ammonium bromide surfactants

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P-113

Computer Assisted Design and Synthesis of Thiazole Based Molecules as Anticancer Agents

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Anticancer drugs are top most selling drugs worldwide. With the emergence of chemoresistance and vast cancer types, quest to design novel and potent anticancer molecules is always a priority.The antiapoptotic Bcl-2[Frenzel et al] proteins are significantly altered in several tumor types positioning them as striking targets for therapeutic intervention. Here we designed, synthesized, computationally validated and biologically evaluated structurally optimized thiazole based small molecules. The virtually designed molecules were subjected to rigorous docking [Ferreira et al] and ADMET studies. Several thiazole based scafolds were designed in 3 steps (up to 80% yield), utilising cheap and readily available starting materials. The molecules were in vitro evaluated against Bcl-2-Jurkat, A-431cell lines and ARPE-19 cell lines which represents human Bcl-2, epidermoid carcinoma and normal cells respectively. Among them molecules **32**, **50**, **53**, **57** are **59** showed potent activities against Bcl-2 Jurkat cell line at concentrations ranging from 32-46 µM respectively. The molecule **32** emerged as most potent and was subjected to molecular dynamics (MD) [Kumari et al] simulation with death defying anti-apoptotic Bcl-2 proteins (4IEH). It was shown that **32** interacted with protein majorly via hydrophobic interactions and few electrostatic interactions were also observed. [Pang et al]During the MD simulation conformational changes in Bcl-2 protein was observed that facilitates the movement of ligand inside the cavity of protein (majorly involving α3, α4, α5, helices) Flow cytometry analysis of compound **32** suggested that cell undergoes 87.66% Annexin A5 positive. It was proved that cell followed apoptotic pathway leading to cell death. All the information starting from design and synthesis of these molecules will be presented in the poster.

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P-114

Adsorption of some Styrylpyridinium dyes on Unmodified and Graphene-modified Silica surface

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ABSTRACT: Adsorption of some styryl pyridinium dyes bearing different alkyl chain length and varying substituents has been carried out on unmodified as well as graphene-modified silica from organic solvents of varying polarities. The morphology study of both unmodified and graphene-modified silica (GMS) were performed employing Scanning Electron Microscope (SEM) and Dynamic Light Scattering (DLS) techniques. The influence of contact time, adsorbent dosages, concentration of dyes and temperature on dye adsorption has been determined. The kinetics of adsorption have been studied and mechanism of adsorption has been proposed. The comparative adsorptivity capacity of both adsorbents were investigated which enlightens the solute-solvent and solute-silica surface interactions in different organic solvents. The data were fitted to Langmuir and Freundlich adsorption isotherms to ascertain the best fit. The influence of alkyl chain of the dye molecules on the formation of layers on silica surface has been investigated. The thermodynamic parameters have been analyzed to understand the feasibility of adsorption phenomena of dyes on unmodified and graphene-modified silica surfaces in organic solvents. The phenomenon of solvation of the dye molecules in the organic solvents has been correlated with the extent of their adsorption on the silica surfaces.

P-115

Direct Regio and Stereospecific N-Me Aziridination of Olefins

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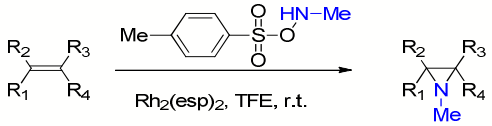
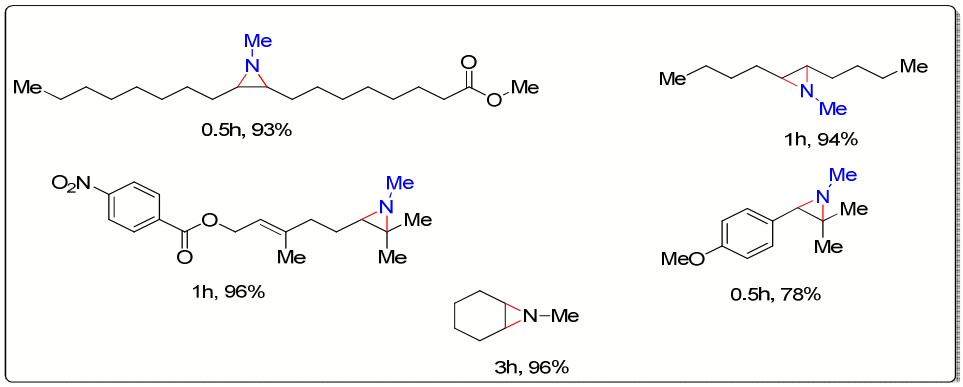
Aziridines are important substructures of biologically active natural products and pharmaceuticals. Their high reactivity towards ring opening, ring expansionand rearrangements make them as a useful synthetic intermediate. The syntheses of activated aziridines from alkenes are well established while the direct methods for non-activated aziridines are less explored. Herein we describe the highly efficient direct method for regioand stereospecific synthesis of N-Me aziridines from olefins in a single stepby using O-(sulfonyl) hydroxylamine as the aminating agent, di-rhodium catalyst in 2,2,2-trifluoroethanol(TFE) as a solvent [1].





Selected examples of N-Me Aziridines

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P-116

Direct Synthesis of Amides from Ketonesthrough Beckmann Rearrangement

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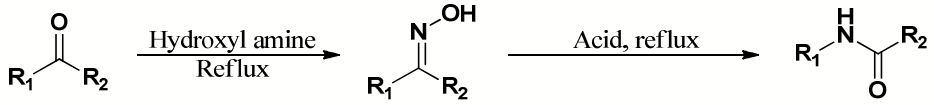
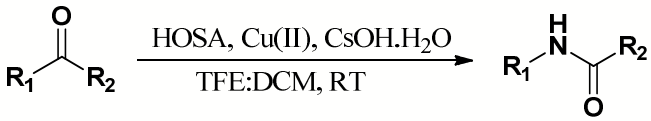
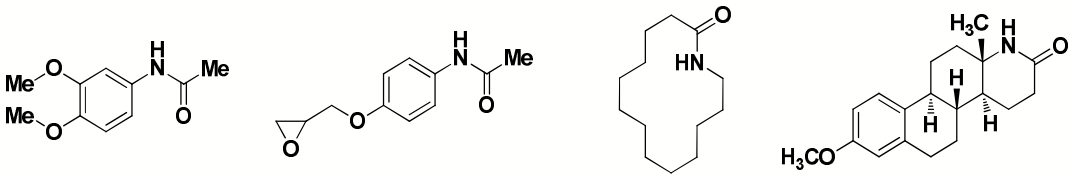
Amides are one of the most important functional group in nature and constitute versatile building blocks in synthetic organic chemistry and exhibit a great interest in industrial and pharmacological area[1]. Beckmann rearrangement (BKR) is an excellent method to synthesize amides from ketoximes. The traditional BKR require high temperature and strong acidic medium which cannot be used for sensitive groups[2].There are rare reports to synthesize amides directly from ketones under milder condition. Herein we report a copper catalyzed single step, one pot synthesis of amides from ketones by using HOSA reagent and Cs(OH).H_2O as base in TFE:DCM [3].

Synthesis of amide from ketone through Beckmann Rearrangement:



Direct synthesis of amide from ketone(Our Work):





rt, 18h, 80% | rt, 16h, 75% | rt, 17 h, 89% | rt, 22h, 85%

Selected Examples

References:

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3. Unpublished results, Manuscript under communication.

P-117

Unexpected Formation of 7-Aryldibenzo[*c,h*]acridines from Donor-Acceptor Cyclopropanes and 1-Naphthylamine

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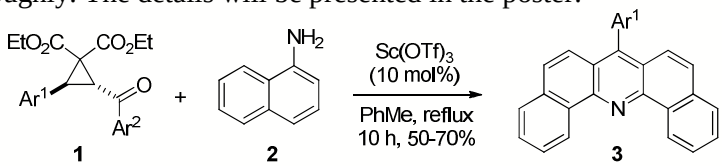
Acridines are important heterocyclic compounds that have attracted considerable attention in synthetic chemistry owing to their wide range of biological and material science applications [1]. Although many methods are available for the synthesis of substituted acridines, only few methods exist for the access of benzo-fused acridines (which are promising OLED materials) [2]. The reported syntheses often involve multistep procedures and as a consequence, commercially available benzo-fused acridines are very expensive. Donor-Acceptor (D-A) cyclopropanes are one of the fascinating building blocks in organic synthesis and a plethora of carbocycles, heterocycles and natural products could be synthesized through various reactions of these cyclopropanes [3]. In continuation our interest in exploring the synthetic potential of aroyl substituted D-A cyclopropanes [4], we investigated their ring opening reactions with various amines. During the course of the study, we found that when D-A cyclopropanes **1** were heated under reflux with 1-naphthylamine (**2**) in the presence of a catalytic amount of scandium(III) triflate, 7-aryldibenzo[*c,h*]acridines **3** were produced in good yields (**Scheme-1**), instead of expected quinolines. The unexpected formation of dibenzoacridines in a single step prompted us to investigate the mechanism and substrate scope of the transformation thoroughly. The details will be presented in the poster.



Scheme-1

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P-118

Synthesis, characterization and biological evolution of novel biphenylic dihydropyrimidine derivatives of pharmacological importance

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Abstract: It is evident from the literature that dihydropyrimidine derivatives exhibit a broad range of biological activities such as anticancer, antiviral, antibacterial, antioxidant, anti-inflammatory etc. Looking to the pharmacological importance of dihydropyrimidinemoiety,we have synthesized some novel dihydropyrimidine derivatives in the present study. Seven different β-Keto esters (i.e. ethylacetoacetate, acetoacetanilide, 2,6-dimethylacetoacetanilide, methyl acetoacetate, ethylcyanoacetate, 3-methyl-5-pyrazolone and 1-phenyl, 3-methyl-5-pyrazolone) were treated with urea or thiourea along withbiphenyl carbaldehyde derivativesusing DMSO as solvent to form different biphenylic dihydropyrimidine derivatives. Structures of the newly synthesized compoundswereanalysed by IR,^{1}H NMR and Mass spectrometry. The compounds were tested for antibacterial and antifungal activity.

P-119

Discovery of N-(4-Chlorophenyl)-4-Oxo-4-Phenylbutanamides for the Treatment of Alzheimer's disease

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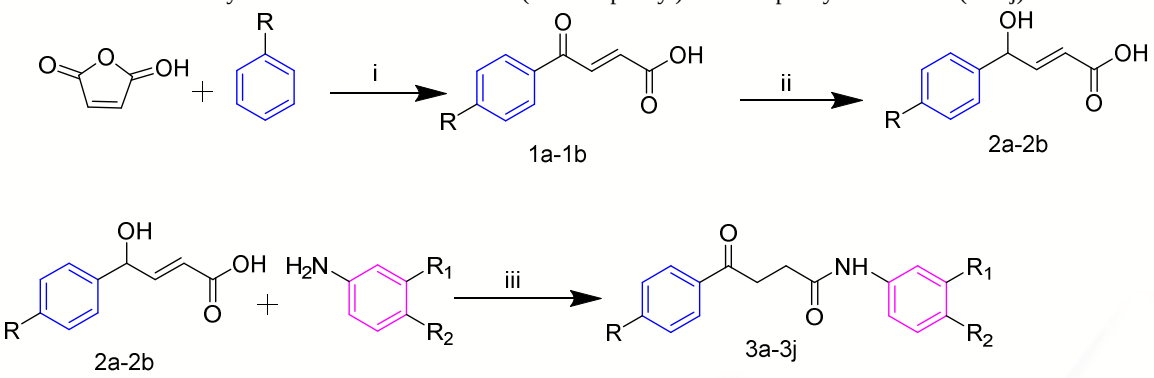
Alzheimer's disease (AD) is a multifactorial, irreversible neurodegenerative disorder of the central nervous system (CNS), which is associated with progressive memory loss, language skills decline and other cognitive impairments resulting in death. Large number of extraneuronalneuritic amyloid (Aβ) plaques and intraneuronal hyperphosphorylated tau proteins, containing neurofibrillary tangles (NFT) in the neocortex and hippocampus are the main characteristic hallmarks of AD. Fragment based drug design approach was utilized for design molecules for synthesis. The ligand-protein interactions, using molecular docking studies were helped to select molecules for synthesis. Para substituted N-(4-chlorophenyl)-4-oxo-4-phenylbutanamide derivatives were synthesized by reacting para-substituted (E)-4-hydroxy-4-phenylbut-2-enoic acid with different aromatic amines in presence of 1-Ethyl-3-(3-dimethylaminopropyl)carbodiimide (EDCI), hydroxybenzotriazole (HOBt) and acetonitrile at room temperature for 16hrs. The synthesized compounds were purified and characterized by spectral analysis including 1H-NMR, 13C-NMR and MS. The synthesized compounds were successfully evaluated for their *in vitro* inhibitory action against cholinesterase and mono amino oxidase. The compounds 3a and 3i were found to be the most potent enzymes inhibitions activities, (e.g. IC_{50} values for AChE were 0.13±0.14µM and 0.24±0.02 µM respectively) and may be considered as lead for treatment of AD.

Scheme: Synthesis of Para substituted N-(4-chlorophenyl)-4-oxo-4-phenyl butanamide(3a-3j):



i)$AlCl_3$, dry DCM, reflux,30-35°C,24 hrs, yield 70-80%. ii) Sodium borohydride,$NaHCO_3$, rt, stirring, overnight, yield 80-90%. iii)1-Ethyl-3-(3-dimethylaminopropyl)carbodiimide (EDCI) and hydroxybenzotriazole(HOBt), ACN, rt, 16hrs, yield 45-78%.

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P-120

Immunomodulatory Effect of Cynodon Dactylon Fractions In Female Mice: A Study For Regulation Of Estrogen Activity And Cure Of PCOS (Polycystic Ovarian Syndrome)

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Cynodon dactylon juice has been traditionally and extensively used as a tonic and as powder for several ailments. *C. dactylon* has been employed in the treatment of cancer, anti-inflammatory, diuretic, antidiabetic, hypolipidemic, and hepatoprotective effects and also to prevent vomiting and burning sensation, hallucinations and fever. Several reports that exist on the extraction and identification of *C. dactylon* constituent compounds point to C-glycosides, apigenin, luteolin, beta sitosterol, citronellol, phytol, linoleniec acid, docosanoic acid, syringol, hexadecanoic acid, eicosanoic acid and truxillic acid. Biological activity and properties of the extracts of *C. dactylon* in diabetes, cancer, CNS activity and kidney stone formation have been reported. However, the active compounds and their mechanism of action have not been ascertained through the studies reported so far.

Polycystic ovary syndrome (PCOS) is characterized by oligo-anovulation, clinical or biochemical hyperandrogenism and/or polycystic ovaries. The condition affects 5-10% of women during reproductive age. There appears to be four times greater incidence of metabolic syndrome association in south-Asian population than in Caucasian counterparts. Treatment of PCOS has limited drugs like metformin either alone or in combination with clomiphene citrate is most widely used insulin-sensitizer for ovulation induction in women with PCOS. The rationale of this treatment was based on only a few small studies with conflicting results. Current treatment options e.g. oral contraceptives (OCs), lifestyle modification, and insulin sensitizers are not considered satisfactory by most gynaecologists. Therefore there is strong need of alternative therapies for PCOS

.

We have very strong ancient wisdom of Ayurveda; therefore in search of an effective alternative herbal therapeutic for PCOS we selected *C. dactylon*. There are other herbs described, which aid the bleeding and clotting mechanisms, these are termed as Raktpitta hara. Therefore, utilizing this vast literature the biological effects of fractions from *Cynodon dactylon* will be evaluated and is expected to provide immunomodulatory effects on experimental model for poly cystic ovarian syndrome. This work establishes *C. dactylon* extract as a potential modulator for PCOS thus enabling a possibility of this plant extract as a new alternative to existing malicious therapy for PCOS affecting millions of females worldwide.

P-121

"SYNTHESIS AND ANTIMICROBIAL ACTIVITY OF SOME 1,3,4-OXADIAZOLE DERIVATIVES"

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Abstract: A series of novel 1, 3, 4-oxadiazole derivatives were efficiently synthesized and characterized by IR, ^{1}H NMR, ^{13}C NMR spectroscopy and mass spectrometry. The newly synthesized *N*'-(1-(2-methyl-2-phenyl-5-(pyridin-4-yl)-1,3,4-oxadiazol-3(2*H*)-yl)ethylidene)benzohydrazides were evaluated for their *in vitro* antimicrobial activity against four bacterial stains like *Staphylococcus aureus* (MTCC-96), *Streptococcus pyogenes* (MTCC-442), *Escherichia coli* (MTCC-443), *Pseudomonas aeruginosa* (MTCC-1688, and three fungal *Candida albicans*(MTCC 227), *Aspergillus niger* (MTCC 282), *A. clavatus*(MTCC 1323) by using conventional broth micro dilution method. We observed that the presence of electron withdrawing groups at para position of phenyl ring enormously enhanced the antibacterial activity. From the results, they were found to possess excellent antimicrobial activity. The antimicrobial screening data revealed that selected screened compounds exhibited significant activity against all microbial and fungal strains.

P-122

"ANTIMICROBIAL EVALUATION OF SOME NOVEL PYRAZOLE CLUBBED 1,3,4-OXADIAZOLE HETEROCYCLES"

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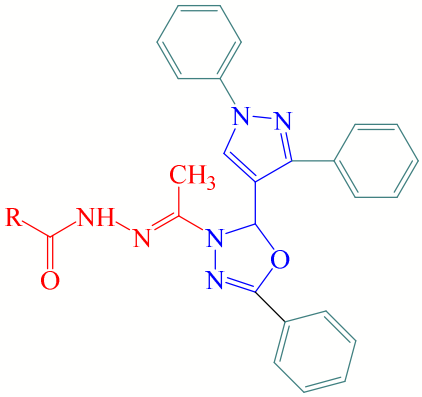
It was found that pyrazole and oxadiazole moieties played a vital role for the development of antimicrobialagents. In search of new pyrazole and oxadiazole containing compounds, we have synthesized *N'*-(1-(2-(1,3-diphenyl-1-*H*-pyrazole-4-yl)-5-phenyl-1,3,4-oxadiazole-3(2*H*)-yl)ethylidene)-(aryl)-benzohydrazidesby combining 1,3,4-oxadiazole and pyrazole scaffolds having diverse pharmacological activities. All the newly synthesized compounds werecharacterized by different analytical techniques like IR, ^{1}H and ^{13}C NMR and mass spectrometry. These compounds have been evaluated for their *in vitro* antimicrobial activity against Gram-positive bacteria *Staphylococcus aureus* (MTCC 96), *Streptococcus pyogenes* (MTCC 442), Gram-negative bacteria *Escherichia coli* (MTCC 443),*Pseudomonas aeruginosa* (MTCC 1688), fungi *Candida albicans* (MTCC 227), *Aspergillus niger* (MTCC 282) and *Aspergillus clavatus* (MTCC 1323) using serial broth dilution method. From the results, it was found that compounds with electron withdrawing groups showed excellent antibacterial activity while compounds with electron donating group showed very good antifungal activity.



P-123

"SYNTHESIS AND ANTIMICROBIAL EVALUATION OF SOME 4-THIAZOLIDINONE DERIVATIVESBEARING QUINAZOLINE HYBRID"

Keyur Shah, Prashant N Shihora& N C Desai*

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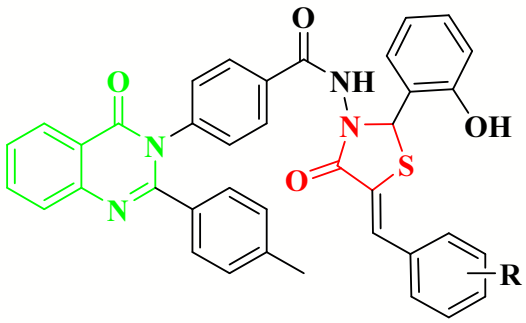
Two different heterocycles moieties quinazoline and 4-thiazolidinone are biologically important, and due to this reason, we have clubbed for synthesizing a novel series of N-(2-(2-hydroxyphenyl)-5-(aryl)-4-oxothiazolidin-3-yl)-4-(4-oxo-2-(p-tolyl)quinazolin-3(4H)-yl)benzamides (4a-n). Structural identificationswere accomplished by using IR, ^{1}H NMR, ^{13}C NMR and Mass spectrometry. All these compounds were screened for their antibacterial activity against Escherichia coli (MTCC 443), Pseudomonas aeruginosa (MTCC 1688), Staphylococcus aureus (MTCC 96), Streptococcus pyogenes (MTCC 442) as well as antifungal activity against Candida albicans (MTCC 227), Aspergillus niger (MTCC 282) and Aspergillus clavatus (MTCC 1323). From the screened results, it has been observed that compounds containing electron withdrawing group showed promising antibacterial and antifungal activity.



Where R = Different Substituent

P-124

"SYNTHESIS, ANTIMICROBIAL AND ANTIFUNGAL EVALUATION OF NOVEL 1, 3, 4 – OXADIAZOLE ANALOGUES"

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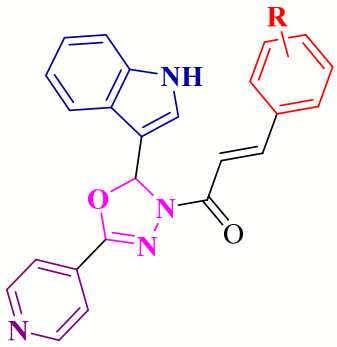
1, 3, 4-oxadiazole derivatives were efficiently synthesized and characterized by different spectroscopy methods. Novel 1-(2-(1*H*-indol-3-yl)-5-(pyridin-4-yl)-1,3,4-oxadiazol-3(2*H*)-yl)-3-(aryl) prop-2-en-1-ones were synthesized and screened for *in-vitro* antimicrobial activity against four bacterial stains i.e. *Staphylococcus aureus*(Gram-positive) (MTCC-96), *Streptococcus pyogenes* (Gram-positive) (MTCC-442),*Escherichia coli* (Gram-negative) (MTCC-443), *Pseudomonas aeruginosa* (Gram-negative) (MTCC-1688) and antifungal activity against three fungi *Candida albicans* (MTCC-227), *Aspergillus niger* (MTCC-282), *Aspergillus clavatus*(MTCC-1323) by Serial broth dilution technique. We observed that the presence of electron withdrawing groups at para position of phenyl ring enormously enhanced the antibacterial activity. From the results, they were found to possess excellent antimicrobial activity. The antimicrobial screening data revealed that selected screened compounds exhibited significant activity against all bacterial and fungal strains.



P-125

Role of nitric oxide in age related neurodegenerative diseases: Insights in CNS pathologies

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Abstract - Nitric oxide (NO) is a pleiotropic ambidextrous molecule synthesized by nitric oxide synthases (NOS) which plays a critical role in a number of physiological and pathological processes in CNS. The physiological roles of NO depend on its local concentrations as well as its downstream target molecule. It could also act as neurotransmitter depending on its concentration and modulates the inflammatory process acting on key regulatory pathways involving excitotoxicity, induced by glutamate accumulation. Excessive NO production evoked the various signaling mechanisms like inflammatory reactions, activation of microglia and astrocytes, damage to the mitochondrial electron transport chain and thus induction of neuronal apoptosis. NO reversibly bind to mitochondrial cytochrome oxidase and compete for oxygen, resulting in inhibition of energy production and sensitization to hypoxia. In addition NO can be converted to a number of reactive derivatives such as peroxynitrite, NO_2, $N2O_3$, and S-nitrosothiols that can kill cells in part by inhibiting mitochondrial respiration or activation of mitochondrial permeability transition, triggering neuronal apoptosis or necrosis. Glial nitric oxide could also contribute to neuronal apoptosis as neuronal-glia synergism is very well known for maintaining neuronal physiology specifically in cellular pool of antioxidants. However, it could also offer neuroprotection through S-nitrosylation. It offers protection against excitotoxicity by S-nitrosylating the NR1 and NR2 subunits of the NMDA receptor thus reducing the intracellular Ca^{2+} influx that is responsible for neuronal death. S-nitrosylation has also been shown to reduce the activity of caspases as observed in several cell lines, including neurons. This chapter appraise about the diverse role of NO during neurodegenerative and neuroprotective mechanisms that may be useful in the prediction of new therapeutic targets for age related neurodegenerative diseases.

P-126

1H NMR urine metabolomics is an effective prognostic indicator in acute spinal cord injury (ASCI) cases: A prospective case control study

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Introduction: Acute spinal cord injury (ASCI) is an extremely devastating disease with high morbidity and mortality. Despite major successes in understanding the pathophysiology of ASCI, little is known about limiting the neurological damage and predicting recovery. Biofluids metabolomics by ^{1}H NMR spectroscopy have provided a window of opportunities for quantification of metabolites specific to nervous tissue injury.

Objective: To evaluate the derangements of urinary metabolic profile in ASCI cases on two different modalities of treatment.

Materials and Methods: Seventy participants were enrolled as *"healthy control"* (Group-1). Seventy ASCI cases were divided equally into two groups as per treatment strategy. Group-2 had "*fixation with stem cells therapy"* and Group-3 "*fixation alone*". Urine samples were collected at baseline, after surgery 6th week, 3rd and at 6th month for ^{1}H NMR spectroscopic measurements. The spectra were subjected to multivariate Orthogonal Partial Least Square Discriminant Analysis (OPLS-DA) and Variable Importance to the Projection (VIP) analysis. The significant metabolites were correlated with neurological recovery.

Results: An OSC-PCA and OPLS-DA model for investigating the role of metabolites emerging from final follow-up data were found to be acetate, creatine, creatinine, creatine phosphate, phenylalanine and urea. It was further substantiated on *VIP score* plots. The 3D scattered score plots in OPLS-DA represented the shifting of more cases towards control group in the final follow-up.

Conclusion: These metabolic aberrations observed between metabolite levels in urine and disease severity at any given time following ASCI could be a potential biomarker or a predictor of neurological recovery.

Keywords: Metabolomics, NMR spectroscopy, acute spinal cord injury (ASCI), Thoraco-lumbar Injury Severity Scale and Score (TLISS), Asia impairment scale (AIS).

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